Ruthenium dihydride and hydride fluoride complexes with N-heterocyclic carbenes: A route to C-F bond activation

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Foreword

This file contains the full crystallographic data for all compounds in this thesis that have been characterised by X-ray crystallography.

Contents

Table 1. Crystal data and structure refinement for $Ru(PPh_3)_3(CO)HF$ **(1)**.

Compound	$Ru(PPh_3)_3(CO)HF$ **(1)**
Empirical formula	C59 H54 F O2 P3 Ru
Formula weight	1008.00
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	Pn
Unit cell dimensions	a = 12.9570(2)Å α = 90°
	b = 12.4210(2)Å β = 96.749(1)°
	c = 15.1290(2)Å γ = 90°
Volume	2417.97(6) $Å^3$
Z	2
Density (calculated)	1.384 Mg/m^3
Absorption coefficient	0.471 mm^{-1}
F(000)	1044
Crystal size	0.30 x 0.25 x 0.20 mm
Theta range for data collection	3.95 to 27.49 °.
Index ranges	-16<=h<=16; -16<=k<=16; -19<=l<=19
Reflections collected	50166
Independent reflections	10639 [R(int) = 0.0341]
Reflections observed (>2σ)	9833
Data Completeness	0.992
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.91 and 0.88
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10639 / 3 / 600
Goodness-of-fit on F^2	1.035
Final R indices [I>2σ(I)]	R1 = 0.0254 wR2 = 0.0581
R indices (all data)	R1 = 0.0303 wR2 = 0.0604
Absolute structure parameter	-0.054(14)
Largest diff. peak and hole	0.678 and -0.505 $eÅ^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(PPh_3)_3(CO)HF$ **(1)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	2012(1)	7523(1)	4852(1)	20(1)
P(1)	1996(1)	9424(1)	4852(1)	22(1)
F(1)	797(1)	7749(1)	3822(1)	32(1)
O(1)	3681(1)	7214(1)	6361(1)	37(1)
C(1)	3031(2)	7327(2)	5772(2)	27(1)
P(2)	3278(1)	7115(1)	3824(1)	21(1)
C(2)	2875(2)	10155(2)	5688(2)	27(1)
P(3)	1158(1)	5877(1)	4990(1)	23(1)
C(3)	3417(2)	11088(2)	5529(2)	35(1)
C(4)	4008(2)	11611(2)	6219(2)	41(1)
C(5)	4056(2)	11243(2)	7081(2)	41(1)
C(6)	3487(2)	10331(2)	7256(2)	39(1)
C(7)	2912(2)	9788(2)	6558(2)	32(1)
C(8)	735(2)	9929(2)	5117(1)	27(1)
C(9)	647(2)	10972(2)	5442(2)	35(1)

C(10)	-305(2)	11345(2)	5649(2)	44(1)
C(11)	-1171(2)	10691(2)	5534(2)	48(1)
C(12)	-1097(2)	9660(2)	5195(2)	46(1)
C(13)	-151(2)	9280(2)	4985(2)	36(1)
C(14)	2090(2)	10078(2)	3777(1)	25(1)
C(15)	1176(2)	10248(2)	3203(1)	27(1)
C(16)	1217(2)	10639(2)	2344(1)	32(1)
C(17)	2161(2)	10873(2)	2056(2)	36(1)
C(18)	3071(2)	10700(2)	2612(2)	35(1)
C(19)	3043(2)	10306(2)	3467(2)	30(1)
C(20)	4381(2)	8066(2)	3854(2)	26(1)
C(21)	4788(2)	8530(2)	4666(2)	31(1)
C(22)	5601(2)	9268(2)	4694(2)	37(1)
C(23)	6013(2)	9564(2)	3924(2)	41(1)
C(24)	5608(2)	9118(2)	3121(2)	38(1)
C(25)	4798(2)	8377(2)	3088(2)	32(1)
C(26)	3956(2)	5831(2)	4081(1)	24(1)
C(27)	4888(2)	5781(2)	4634(2)	31(1)
C(28)	5350(2)	4798(2)	4879(2)	36(1)
C(29)	4870(2)	3850(2)	4583(2)	38(1)
C(30)	3943(2)	3881(2)	4033(2)	34(1)
C(31)	3487(2)	4862(2)	3779(1)	29(1)
C(32)	2867(2)	7017(2)	2626(1)	23(1)
C(33)	3327(2)	6320(2)	2060(1)	27(1)
C(34)	3010(2)	6333(2)	1151(1)	29(1)
C(35)	2257(2)	7052(2)	795(1)	29(1)
C(36)	1791(2)	7746(2)	1357(2)	28(1)
C(37)	2089(2)	7719(2)	2271(2)	26(1)
C(38)	-196(2)	6149(2)	5195(1)	27(1)
C(39)	-382(2)	6521(2)	6031(2)	34(1)
C(40)	-1381(2)	6752(2)	6211(2)	39(1)
C(41)	-2210(2)	6647(2)	5544(2)	39(1)
C(42)	-2026(2)	6302(2)	4712(2)	40(1)
C(43)	-1023(2)	6047(2)	4544(2)	33(1)
C(44)	1640(2)	4961(2)	5897(1)	28(1)
C(45)	2692(2)	4810(2)	6080(2)	30(1)
C(46)	3094(2)	4089(2)	6742(2)	37(1)
C(47)	2421(2)	3520(2)	7220(2)	41(1)
C(48)	1364(2)	3667(2)	7038(2)	42(1)
C(49)	971(2)	4378(2)	6377(2)	36(1)
C(50)	996(2)	4969(2)	4027(2)	28(1)
C(51)	1102(2)	3860(2)	4118(2)	39(1)
C(52)	1057(2)	3205(2)	3367(2)	46(1)
C(53)	899(2)	3654(2)	2529(2)	46(1)
C(54)	756(2)	4757(2)	2436(2)	38(1)
C(55)	815(2)	5421(2)	3174(2)	32(1)
C(56)	7089(3)	3549(3)	3106(3)	81(1)
C(57)	6668(3)	2422(3)	3067(3)	63(1)
O(58)	7416(2)	1769(2)	3547(2)	63(1)
C(59)	8395(3)	2260(3)	3479(2)	56(1)
C(60)	8203(3)	3444(3)	3478(2)	67(1)

Table 3. Bond lengths [Å] and angles [°] for $Ru(PPh_3)_3(CO)HF$ **(1)**.

Ru(1)-C(1)	1.819(3)	Ru(1)-F(1)	2.0986(15)
Ru(1)-P(3)	2.3462(5)	Ru(1)-P(1)	2.3608(5)
Ru(1)-P(2)	2.4422(5)	P(1)-C(14)	1.835(2)
P(1)-C(8)	1.838(2)	P(1)-C(2)	1.839(2)
O(1)-C(1)	1.160(3)	P(2)-C(32)	1.832(2)
P(2)-C(26)	1.840(2)	P(2)-C(20)	1.850(2)
C(2)-C(7)	1.390(3)	C(2)-C(3)	1.390(3)
P(3)-C(50)	1.835(2)	P(3)-C(44)	1.835(2)
P(3)-C(38)	1.848(2)	C(3)-C(4)	1.382(3)
C(4)-C(5)	1.376(4)	C(5)-C(6)	1.393(4)
C(6)-C(7)	1.393(3)	C(8)-C(9)	1.395(3)
C(8)-C(13)	1.397(3)	C(9)-C(10)	1.387(4)
C(10)-C(11)	1.379(4)	C(11)-C(12)	1.388(4)
C(12)-C(13)	1.385(3)	C(14)-C(15)	1.399(3)
C(14)-C(19)	1.400(3)	C(15)-C(16)	1.394(3)
C(16)-C(17)	1.378(3)	C(17)-C(18)	1.381(4)
C(18)-C(19)	1.387(3)	C(20)-C(25)	1.390(3)
C(20)-C(21)	1.402(3)	C(21)-C(22)	1.394(3)
C(22)-C(23)	1.387(4)	C(23)-C(24)	1.382(4)
C(24)-C(25)	1.392(3)	C(26)-C(27)	1.387(3)
C(26)-C(31)	1.400(3)	C(27)-C(28)	1.390(3)
C(28)-C(29)	1.381(4)	C(29)-C(30)	1.380(3)
C(30)-C(31)	1.388(3)	C(32)-C(37)	1.393(3)
C(32)-C(33)	1.399(3)	C(33)-C(34)	1.388(3)
C(34)-C(35)	1.384(3)	C(35)-C(36)	1.396(3)
C(36)-C(37)	1.391(3)	C(38)-C(43)	1.373(3)
C(38)-C(39)	1.393(3)	C(39)-C(40)	1.385(3)
C(40)-C(41)	1.391(4)	C(41)-C(42)	1.377(4)
C(42)-C(43)	1.390(3)	C(44)-C(45)	1.372(3)
C(44)-C(49)	1.396(3)	C(45)-C(46)	1.397(3)
C(46)-C(47)	1.390(4)	C(47)-C(48)	1.377(4)
C(48)-C(49)	1.386(4)	C(50)-C(51)	1.389(3)
C(50)-C(55)	1.400(3)	C(51)-C(52)	1.393(3)
C(52)-C(53)	1.378(4)	C(53)-C(54)	1.387(4)
C(54)-C(55)	1.383(3)	C(56)-C(60)	1.492(6)
C(56)-C(57)	1.500(5)	C(57)-O(58)	1.401(4)
O(58)-C(59)	1.422(4)	C(59)-C(60)	1.492(4)
C(1)-Ru(1)-F(1)	177.94(11)	C(1)-Ru(1)-P(3)	97.02(8)
F(1)-Ru(1)-P(3)	82.06(4)	C(1)-Ru(1)-P(1)	98.04(8)
F(1)-Ru(1)-P(1)	82.00(5)	P(3)-Ru(1)-P(1)	150.13(2)
C(1)-Ru(1)-P(2)	88.76(8)	F(1)-Ru(1)-P(2)	93.25(4)
P(3)-Ru(1)-P(2)	103.579(19)	P(1)-Ru(1)-P(2)	102.40(2)
C(14)-P(1)-C(8)	101.28(10)	C(14)-P(1)-C(2)	106.90(10)
C(8)-P(1)-C(2)	100.16(10)	C(14)-P(1)-Ru(1)	116.16(7)
C(8)-P(1)-Ru(1)	110.46(7)	C(2)-P(1)-Ru(1)	119.27(8)
O(1)-C(1)-Ru(1)	179.2(2)	C(32)-P(2)-C(26)	103.14(9)
C(32)-P(2)-C(20)	101.58(9)	C(26)-P(2)-C(20)	101.56(10)
C(32)-P(2)-Ru(1)	120.30(7)	C(26)-P(2)-Ru(1)	112.66(7)
C(20)-P(2)-Ru(1)	115.22(7)	C(7)-C(2)-C(3)	118.4(2)
C(7)-C(2)-P(1)	116.05(17)	C(3)-C(2)-P(1)	125.25(18)
C(50)-P(3)-C(44)	102.10(10)	C(50)-P(3)-C(38)	102.93(10)
C(44)-P(3)-C(38)	103.52(10)	C(50)-P(3)-Ru(1)	118.43(8)

C(44)-P(3)-Ru(1)	118.98(7)	C(38)-P(3)-Ru(1)	108.83(7)
C(4)-C(3)-C(2)	120.5(2)	C(5)-C(4)-C(3)	121.2(2)
C(4)-C(5)-C(6)	119.0(2)	C(5)-C(6)-C(7)	119.9(2)
C(2)-C(7)-C(6)	121.0(2)	C(9)-C(8)-C(13)	119.1(2)
C(9)-C(8)-P(1)	120.37(18)	C(13)-C(8)-P(1)	120.56(16)
C(10)-C(9)-C(8)	120.1(2)	C(11)-C(10)-C(9)	120.5(2)
C(10)-C(11)-C(12)	120.0(2)	C(13)-C(12)-C(11)	120.0(3)
C(12)-C(13)-C(8)	120.4(2)	C(15)-C(14)-C(19)	118.47(19)
C(15)-C(14)-P(1)	118.50(16)	C(19)-C(14)-P(1)	122.66(17)
C(16)-C(15)-C(14)	120.6(2)	C(17)-C(16)-C(15)	120.0(2)
C(16)-C(17)-C(18)	120.0(2)	C(17)-C(18)-C(19)	120.6(2)
C(18)-C(19)-C(14)	120.3(2)	C(25)-C(20)-C(21)	118.2(2)
C(25)-C(20)-P(2)	122.13(17)	C(21)-C(20)-P(2)	119.59(17)
C(22)-C(21)-C(20)	120.1(2)	C(23)-C(22)-C(21)	120.9(2)
C(24)-C(23)-C(22)	119.2(2)	C(23)-C(24)-C(25)	120.2(2)
C(20)-C(25)-C(24)	121.3(2)	C(27)-C(26)-C(31)	118.14(19)
C(27)-C(26)-P(2)	121.74(17)	C(31)-C(26)-P(2)	119.89(16)
C(26)-C(27)-C(28)	121.1(2)	C(29)-C(28)-C(27)	119.9(2)
C(30)-C(29)-C(28)	119.9(2)	C(29)-C(30)-C(31)	120.2(2)
C(30)-C(31)-C(26)	120.7(2)	C(37)-C(32)-C(33)	119.48(19)
C(37)-C(32)-P(2)	116.96(15)	C(33)-C(32)-P(2)	123.48(16)
C(34)-C(33)-C(32)	120.1(2)	C(35)-C(34)-C(33)	120.4(2)
C(34)-C(35)-C(36)	119.8(2)	C(37)-C(36)-C(35)	120.1(2)
C(36)-C(37)-C(32)	120.1(2)	C(43)-C(38)-C(39)	118.6(2)
C(43)-C(38)-P(3)	122.57(16)	C(39)-C(38)-P(3)	118.80(18)
C(40)-C(39)-C(38)	120.8(2)	C(39)-C(40)-C(41)	119.9(2)
C(42)-C(41)-C(40)	119.4(2)	C(41)-C(42)-C(43)	120.2(2)
C(38)-C(43)-C(42)	121.0(2)	C(45)-C(44)-C(49)	119.1(2)
C(45)-C(44)-P(3)	118.59(17)	C(49)-C(44)-P(3)	122.23(17)
C(44)-C(45)-C(46)	120.7(2)	C(47)-C(46)-C(45)	119.6(2)
C(48)-C(47)-C(46)	119.9(2)	C(47)-C(48)-C(49)	120.0(2)
C(48)-C(49)-C(44)	120.6(2)	C(51)-C(50)-C(55)	119.5(2)
C(51)-C(50)-P(3)	122.02(18)	C(55)-C(50)-P(3)	118.42(17)
C(50)-C(51)-C(52)	120.3(2)	C(53)-C(52)-C(51)	120.0(3)
C(52)-C(53)-C(54)	119.8(2)	C(55)-C(54)-C(53)	120.8(2)
C(54)-C(55)-C(50)	119.5(2)	C(60)-C(56)-C(57)	105.4(3)
O(58)-C(57)-C(56)	107.1(3)	C(57)-O(58)-C(59)	106.4(3)
O(58)-C(59)-C(60)	105.8(3)	C(56)-C(60)-C(59)	103.9(3)

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(PPh_3)_3(CO)HF$ **(1)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	22(1)	18(1)	19(1)	0(1)	4(1)	0(1)
P(1)	23(1)	19(1)	23(1)	-1(1)	5(1)	0(1)
F(1)	34(1)	35(1)	27(1)	0(1)	3(1)	1(1)
O(1)	40(1)	39(1)	30(1)	1(1)	-5(1)	2(1)
C(1)	33(1)	25(1)	25(1)	-1(1)	8(1)	-2(1)
P(2)	22(1)	21(1)	20(1)	0(1)	3(1)	2(1)
C(2)	27(1)	23(1)	32(1)	-5(1)	5(1)	2(1)
P(3)	25(1)	21(1)	25(1)	-1(1)	5(1)	-1(1)
C(3)	40(1)	26(1)	39(1)	-4(1)	8(1)	-3(1)
C(4)	36(1)	27(1)	60(2)	-12(1)	8(1)	-8(1)

C(5)	35(1)	32(1)	52(2)	-14(1)	-6(1)	2(1)
C(6)	45(1)	36(1)	33(1)	-6(1)	-5(1)	3(1)
C(7)	37(1)	26(1)	33(1)	-2(1)	1(1)	-2(1)
C(8)	34(1)	27(1)	21(1)	2(1)	7(1)	8(1)
C(9)	43(1)	32(1)	30(1)	-3(1)	2(1)	11(1)
C(10)	54(2)	46(2)	33(1)	-4(1)	8(1)	25(1)
C(11)	48(2)	53(2)	48(2)	13(1)	22(1)	28(1)
C(12)	33(1)	47(2)	63(2)	17(1)	18(1)	11(1)
C(13)	33(1)	31(1)	46(1)	4(1)	12(1)	6(1)
C(14)	35(1)	17(1)	24(1)	0(1)	7(1)	2(1)
C(15)	30(1)	23(1)	29(1)	-1(1)	6(1)	1(1)
C(16)	40(1)	27(1)	27(1)	-1(1)	1(1)	3(1)
C(17)	53(2)	29(1)	28(1)	5(1)	10(1)	0(1)
C(18)	39(1)	32(1)	37(1)	3(1)	13(1)	-1(1)
C(19)	33(1)	25(1)	33(1)	2(1)	6(1)	5(1)
C(20)	24(1)	22(1)	31(1)	0(1)	4(1)	2(1)
C(21)	33(1)	31(1)	29(1)	0(1)	2(1)	-1(1)
C(22)	31(1)	40(1)	39(1)	-2(1)	-5(1)	-7(1)
C(23)	32(1)	39(1)	52(2)	1(1)	3(1)	-12(1)
C(24)	36(1)	40(1)	42(1)	2(1)	14(1)	-7(1)
C(25)	32(1)	32(1)	34(1)	-4(1)	10(1)	-1(1)
C(26)	28(1)	23(1)	21(1)	2(1)	6(1)	5(1)
C(27)	31(1)	32(1)	31(1)	-2(1)	2(1)	4(1)
C(28)	34(1)	38(1)	34(1)	2(1)	-2(1)	10(1)
C(29)	41(1)	31(1)	43(1)	9(1)	9(1)	13(1)
C(30)	37(1)	25(1)	41(1)	3(1)	9(1)	1(1)
C(31)	28(1)	28(1)	31(1)	2(1)	7(1)	1(1)
C(32)	23(1)	23(1)	23(1)	-1(1)	4(1)	-3(1)
C(33)	28(1)	26(1)	26(1)	-2(1)	6(1)	0(1)
C(34)	32(1)	30(1)	27(1)	-7(1)	8(1)	-7(1)
C(35)	33(1)	33(1)	22(1)	-1(1)	3(1)	-9(1)
C(36)	26(1)	31(1)	28(1)	4(1)	3(1)	-1(1)
C(37)	23(1)	28(1)	27(1)	-1(1)	5(1)	1(1)
C(38)	26(1)	23(1)	32(1)	0(1)	8(1)	-3(1)
C(39)	31(1)	33(1)	37(1)	-9(1)	5(1)	-6(1)
C(40)	40(1)	40(1)	38(1)	-10(1)	14(1)	-1(1)
C(41)	27(1)	38(1)	54(2)	-3(1)	16(1)	2(1)
C(42)	30(1)	47(1)	41(1)	-1(1)	1(1)	-2(1)
C(43)	31(1)	36(1)	33(1)	-2(1)	8(1)	-1(1)
C(44)	35(1)	21(1)	28(1)	2(1)	6(1)	-1(1)
C(45)	34(1)	21(1)	34(1)	2(1)	6(1)	2(1)
C(46)	40(1)	31(1)	38(1)	1(1)	1(1)	5(1)
C(47)	56(2)	29(1)	37(1)	9(1)	7(1)	8(1)
C(48)	52(2)	36(1)	41(1)	13(1)	14(1)	-4(1)
C(49)	34(1)	35(1)	40(1)	8(1)	6(1)	-3(1)
C(50)	25(1)	28(1)	31(1)	-7(1)	5(1)	-4(1)
C(51)	50(2)	28(1)	40(1)	-6(1)	9(1)	-6(1)
C(52)	56(2)	31(1)	53(2)	-14(1)	11(1)	-5(1)
C(53)	47(2)	50(2)	42(1)	-23(1)	7(1)	-7(1)
C(54)	37(1)	49(2)	29(1)	-9(1)	4(1)	-1(1)
C(55)	29(1)	37(1)	31(1)	-4(1)	5(1)	-1(1)
C(56)	102(3)	60(2)	92(3)	28(2)	60(3)	17(2)
C(57)	64(2)	70(2)	53(2)	-13(2)	7(2)	12(2)
O(58)	62(1)	57(1)	66(1)	19(1)	-4(1)	-19(1)
C(59)	61(2)	66(2)	38(2)	13(1)	-8(1)	-21(2)

C(60)	106(3)	53(2)	46(2)	-11(1)	28(2)	-25(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(PPh_3)_3(CO)HF$ **(1).**

Atom	x	y	z	U(eq)
H(1)	1198(16)	7743(19)	5538(14)	27(6)
H(3)	3380	11369	4942	42
H(4)	4389	12236	6096	49
H(5)	4470	11605	7549	49
H(6)	3493	10080	7849	46
H(7)	2538	9157	6680	39
H(9)	1239	11428	5521	42
H(10)	-361	12055	5871	53
H(11)	-1817	10947	5688	58
H(12)	-1696	9214	5106	56
H(13)	-103	8575	4751	43
H(15)	522	10096	3401	33
H(16)	593	10744	1957	38
H(17)	2188	11154	1475	43
H(18)	3720	10853	2407	42
H(19)	3673	10190	3843	36
H(21)	4508	8340	5198	37
H(22)	5877	9573	5248	45
H(23)	6568	10068	3948	50
H(24)	5883	9317	2589	46
H(25)	4524	8079	2531	38
H(27)	5217	6429	4848	38
H(28)	5994	4779	5250	43
H(29)	5179	3178	4758	45
H(30)	3614	3229	3827	41
H(31)	2851	4876	3397	35
H(33)	3857	5837	2298	32
H(34)	3311	5846	771	35
H(35)	2057	7074	171	35
H(36)	1270	8236	1115	34
H(37)	1760	8181	2653	31
H(39)	185	6619	6482	40
H(40)	-1501	6980	6790	46
H(41)	-2897	6812	5661	47
H(42)	-2587	6239	4250	47
H(43)	-907	5798	3970	40
H(45)	3152	5199	5753	35
H(46)	3824	3989	6864	44
H(47)	2690	3030	7671	49
H(48)	904	3281	7367	51
H(49)	241	4470	6249	43
H(51)	1205	3548	4694	47
H(52)	1136	2447	3432	56
H(53)	888	3210	2017	55
H(54)	616	5060	1858	46
H(55)	734	6177	3104	39
H(56A)	7026	3873	2505	97
H(56B)	6708	4005	3496	97

H(57A)	6006	2393	3333	75
H(57B)	6537	2176	2442	75
H(59A)	8667	2037	2922	67
H(59B)	8905	2055	3990	67
H(60A)	8322	3741	4089	80
H(60B)	8659	3823	3099	80

Table 6. Crystal data and structure refinement for $Ru(IMe_4)(PPh_3)_2(CO)HF$ **(3)**.

Compound	$Ru(IMe_4)(PPh_3)_2(CO)HF$ **(3)**
Empirical formula	C47 H46 F N2 O P2 Ru
Formula weight	836.87
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 14.6000(1)Å α = 90°
	b = 22.8140(2)Å β = 96.007(1)°
	c = 24.3010(2)Å γ = 90°
Volume	8049.84(11) $Å^3$
Z	8
Density (calculated)	1.381 Mg/m^3
Absorption coefficient	0.512 mm^{-1}
F(000)	3464
Crystal size	0.38 x 0.30 x 0.05 mm
Theta range for data collection	3.53 to 34.95°
Index ranges	-23<=h<=23; -36<=k<=36; -39<=l<=39
Reflections collected	94781
Independent reflections	17581 [R(int) = 0.0513]
Reflections observed (>2σ)	13824
Data Completeness	0.994
Absorption correction	Multiscan
Max. and min. transmission	0.97 and 0.94
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17581 / 13 / 490
Goodness-of-fit on F^2	1.062
Final R indices [I>2σ(I)]	R^1 = 0.0391 wR_2 = 0.0783
R indices (all data)	R^1 = 0.0604 wR_2 = 0.0855
Largest diff. peak and hole	1.014 and -0.700 $eÅ^{-3}$

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement Parameters ($Å^2$ x 10^3) for $Ru(IMe_4)(PPh_3)_2(CO)HF$ **(3)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	4235(1)	1370(1)	5854(1)	17(1)
P(1)	5532(1)	1812(1)	5540(1)	18(1)
P(2)	3062(1)	1078(1)	6388(1)	19(1)
F(1)	3460(1)	2139(1)	5853(1)	23(1)
O(1)	5244(1)	235(1)	5911(1)	31(1)
N(1)	3272(1)	1609(1)	4631(1)	20(1)
N(2)	3185(1)	697(1)	4812(1)	21(1)
C(1)	4852(1)	678(1)	5892(1)	22(1)
C(2)	3510(1)	1213(1)	5041(1)	19(1)

C(3)	2812(1)	1351(1)	4162(1)	24(1)
C(4)	2752(1)	772(1)	4277(1)	25(1)
C(5)	3461(1)	2240(1)	4646(1)	24(1)
C(6)	2501(1)	1688(1)	3653(1)	33(1)
C(7)	2319(2)	279(1)	3943(1)	39(1)
C(8)	3203(1)	129(1)	5087(1)	27(1)
C(9)	5586(1)	1826(1)	4788(1)	21(1)
C(10)	5357(1)	1306(1)	4497(1)	24(1)
C(11)	5302(1)	1291(1)	3924(1)	30(1)
C(12)	5478(1)	1795(1)	3631(1)	34(1)
C(13)	5726(1)	2310(1)	3912(1)	33(1)
C(14)	5777(1)	2325(1)	4489(1)	26(1)
C(15)	6644(1)	1481(1)	5789(1)	21(1)
C(16)	7347(1)	1410(1)	5445(1)	28(1)
C(17)	8223(1)	1238(1)	5666(1)	35(1)
C(18)	8405(1)	1129(1)	6230(1)	36(1)
C(19)	7706(1)	1187(1)	6570(1)	33(1)
C(20)	6830(1)	1362(1)	6351(1)	27(1)
C(21)	5779(1)	2570(1)	5769(1)	21(1)
C(22)	6650(1)	2820(1)	5747(1)	28(1)
C(23)	6836(1)	3384(1)	5947(1)	32(1)
C(24)	6164(1)	3703(1)	6173(1)	34(1)
C(25)	5297(1)	3459(1)	6196(1)	34(1)
C(26)	5106(1)	2893(1)	6000(1)	27(1)
C(27)	2747(1)	1657(1)	6865(1)	26(1)
C(28)	3430(2)	1995(1)	7158(1)	32(1)
C(29)	3202(2)	2413(1)	7541(1)	39(1)
C(30)	2291(2)	2506(1)	7625(1)	44(1)
C(31)	1610(2)	2187(1)	7326(1)	43(1)
C(32)	1832(1)	1763(1)	6949(1)	33(1)
C(33)	3310(1)	447(1)	6851(1)	22(1)
C(34)	3650(2)	526(1)	7400(1)	34(1)
C(35)	3845(2)	50(1)	7750(1)	44(1)
C(36)	3693(2)	-516(1)	7559(1)	36(1)
C(37)	3372(1)	-604(1)	7009(1)	32(1)
C(38)	3190(1)	-128(1)	6655(1)	29(1)
C(39)	1940(1)	901(1)	6010(1)	24(1)
C(40)	1349(1)	459(1)	6156(1)	33(1)
C(41)	539(1)	339(1)	5821(1)	45(1)
C(42)	305(1)	657(1)	5343(1)	46(1)
C(43)	865(1)	1116(1)	5207(1)	39(1)
C(44)	1684(1)	1237(1)	5540(1)	28(1)
C(45)	448(1)	326(1)	7499(1)	43(1)
C(46)	888(2)	-198(2)	7515(1)	45(1)
C(47)	533(2)	-724(2)	7514(1)	61(2)
C(45B)	0(2)	-893(2)	7500(1)	57(2)
C(47A)	821(2)	-539(2)	7513(1)	69(3)
C(46A)	754(2)	69(2)	7524(1)	77(3)
C(45A)	0(2)	355(2)	7500(1)	118(7)

Table 8. Bond lengths [Å] and angles [°] for $Ru(IMe_4)(PPh_3)_2(CO)HF$ **(3)**.

Ru(1)-H(1)	1.6083	C(21)-C(26)	1.393(2)
Ru(1)-C(1)	1.8144(16)	C(21)-C(22)	1.400(2)
Ru(1)-F(1)	2.0887(9)	C(22)-C(23)	1.391(2)

Ru(1)-C(2)	2.1702(16)	C(23)-C(24)	1.381(3)
Ru(1)-P(1)	2.3434(4)	C(24)-C(25)	1.389(3)
Ru(1)-P(2)	2.3499(4)	C(25)-C(26)	1.395(2)
P(1)-C(15)	1.8349(16)	C(27)-C(28)	1.394(3)
P(1)-C(9)	1.8383(16)	C(27)-C(32)	1.394(3)
P(1)-C(21)	1.8389(15)	C(28)-C(29)	1.398(3)
P(2)-C(39)	1.8367(17)	C(29)-C(30)	1.382(3)
P(2)-C(33)	1.8400(16)	C(30)-C(31)	1.377(4)
P(2)-C(27)	1.8474(17)	C(31)-C(32)	1.395(3)
O(1)-C(1)	1.160(2)	C(33)-C(34)	1.387(2)
N(1)-C(2)	1.3635(19)	C(33)-C(38)	1.400(2)
N(1)-C(3)	1.392(2)	C(34)-C(35)	1.391(3)
N(1)-C(5)	1.4641(19)	C(35)-C(36)	1.382(3)
N(2)-C(2)	1.3671(19)	C(36)-C(37)	1.383(3)
N(2)-C(4)	1.395(2)	C(37)-C(38)	1.393(2)
N(2)-C(8)	1.455(2)	C(39)-C(44)	1.395(2)
C(3)-C(4)	1.354(2)	C(39)-C(40)	1.396(2)
C(3)-C(6)	1.488(2)	C(40)-C(41)	1.391(3)
C(4)-C(7)	1.489(2)	C(41)-C(42)	1.382(4)
C(9)-C(14)	1.395(2)	C(42)-C(43)	1.389(3)
C(9)-C(10)	1.402(2)	C(43)-C(44)	1.398(3)
C(10)-C(11)	1.388(2)	C(45)-C(45)#1	1.307(3)
C(11)-C(12)	1.389(3)	C(45)-C(46)	1.355(3)
C(12)-C(13)	1.387(3)	C(46)-C(47)	1.3069
C(13)-C(14)	1.397(3)	C(47)-C(47)#1	1.551(5)
C(15)-C(20)	1.392(2)	C(45B)-C(47A)	1.4427
C(15)-C(16)	1.398(2)	C(45B)-C(47A)#1	1.443(4)
C(16)-C(17)	1.391(3)	C(47A)-C(46A)	1.3910
C(17)-C(18)	1.389(3)	C(46A)-C(45A)	1.2756
C(18)-C(19)	1.386(3)	C(45A)-C(46A)#1	1.276(4)
C(19)-C(20)	1.391(2)		
H(1)-Ru(1)-C(1)	86.7	C(12)-C(13)-C(14)	119.93(17)
H(1)-Ru(1)-F(1)	92.0	C(9)-C(14)-C(13)	120.59(16)
C(1)-Ru(1)-F(1)	175.62(6)	C(20)-C(15)-C(16)	118.94(16)
H(1)-Ru(1)-C(2)	176.5	C(20)-C(15)-P(1)	118.60(12)
C(1)-Ru(1)-C(2)	95.46(6)	C(16)-C(15)-P(1)	122.01(14)
F(1)-Ru(1)-C(2)	85.64(5)	C(17)-C(16)-C(15)	120.30(18)
H(1)-Ru(1)-P(1)	86.5	C(18)-C(17)-C(16)	120.34(18)
C(1)-Ru(1)-P(1)	88.72(5)	C(19)-C(18)-C(17)	119.56(18)
F(1)-Ru(1)-P(1)	95.38(3)	C(18)-C(19)-C(20)	120.3(2)
C(2)-Ru(1)-P(1)	96.25(4)	C(19)-C(20)-C(15)	120.54(17)
H(1)-Ru(1)-P(2)	78.9	C(26)-C(21)-C(22)	118.70(15)
C(1)-Ru(1)-P(2)	96.46(5)	C(26)-C(21)-P(1)	119.68(12)
F(1)-Ru(1)-P(2)	79.18(3)	C(22)-C(21)-P(1)	121.51(12)
C(2)-Ru(1)-P(2)	98.10(4)	C(23)-C(22)-C(21)	120.63(16)
P(1)-Ru(1)-P(2)	164.189(15)	C(24)-C(23)-C(22)	120.34(17)
C(15)-P(1)-C(9)	101.92(7)	C(23)-C(24)-C(25)	119.56(16)
C(15)-P(1)-C(21)	98.57(7)	C(24)-C(25)-C(26)	120.49(17)
C(9)-P(1)-C(21)	104.92(7)	C(21)-C(26)-C(25)	120.26(16)
C(15)-P(1)-Ru(1)	115.62(5)	C(28)-C(27)-C(32)	118.33(16)
C(9)-P(1)-Ru(1)	116.78(5)	C(28)-C(27)-P(2)	120.28(14)
C(21)-P(1)-Ru(1)	116.50(5)	C(32)-C(27)-P(2)	121.38(14)
C(39)-P(2)-C(33)	103.91(8)	C(27)-C(28)-C(29)	120.67(19)
C(39)-P(2)-C(27)	101.75(8)	C(30)-C(29)-C(28)	120.2(2)

C(33)-P(2)-C(27)	102.84(7)	C(31)-C(30)-C(29)	119.63(18)
C(39)-P(2)-Ru(1)	116.76(6)	C(30)-C(31)-C(32)	120.6(2)
C(33)-P(2)-Ru(1)	116.82(5)	C(27)-C(32)-C(31)	120.6(2)
C(27)-P(2)-Ru(1)	112.79(6)	C(34)-C(33)-C(38)	117.93(16)
C(2)-N(1)-C(3)	112.44(13)	C(34)-C(33)-P(2)	120.96(13)
C(2)-N(1)-C(5)	126.89(14)	C(38)-C(33)-P(2)	121.08(13)
C(3)-N(1)-C(5)	120.67(13)	C(33)-C(34)-C(35)	121.16(18)
C(2)-N(2)-C(4)	112.21(13)	C(36)-C(35)-C(34)	120.5(2)
C(2)-N(2)-C(8)	126.16(14)	C(35)-C(36)-C(37)	119.11(18)
C(4)-N(2)-C(8)	121.47(13)	C(36)-C(37)-C(38)	120.51(18)
O(1)-C(1)-Ru(1)	179.37(16)	C(37)-C(38)-C(33)	120.71(17)
N(1)-C(2)-N(2)	102.83(13)	C(44)-C(39)-C(40)	118.93(17)
N(1)-C(2)-Ru(1)	128.20(11)	C(44)-C(39)-P(2)	115.93(12)
N(2)-C(2)-Ru(1)	128.97(11)	C(40)-C(39)-P(2)	125.14(15)
C(4)-C(3)-N(1)	106.29(14)	C(41)-C(40)-C(39)	120.3(2)
C(4)-C(3)-C(6)	130.87(16)	C(42)-C(41)-C(40)	120.6(2)
N(1)-C(3)-C(6)	122.82(15)	C(41)-C(42)-C(43)	119.6(2)
C(3)-C(4)-N(2)	106.23(14)	C(42)-C(43)-C(44)	120.1(2)
C(3)-C(4)-C(7)	131.12(17)	C(39)-C(44)-C(43)	120.33(17)
N(2)-C(4)-C(7)	122.64(15)	C(45)#1-C(45)-C(46)	118.14(14)
C(14)-C(9)-C(10)	118.60(15)	C(47)-C(46)-C(45)	128.49(14)
C(14)-C(9)-P(1)	124.24(12)	C(46)-C(47)-C(47)#1	113.3
C(10)-C(9)-P(1)	117.01(12)	C(47A)-C(45B)-C(47A)#1	111.92(10)
C(11)-C(10)-C(9)	120.81(16)	C(46A)-C(47A)-C(45B)	119.9
C(10)-C(11)-C(12)	119.93(16)	C(45A)-C(46A)-C(47A)	124.9
C(13)-C(12)-C(11)	120.11(18)	C(46A)-C(45A)-C(46A)#1	118.43(11)

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+3/2

Table 9. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IMe_4)(PPh_3)_2(CO)HF$ **(3)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	17(1)	15(1)	17(1)	0(1)	2(1)	0(1)
P(1)	18(1)	16(1)	20(1)	0(1)	3(1)	-1(1)
P(2)	20(1)	18(1)	19(1)	-1(1)	4(1)	-1(1)
F(1)	22(1)	19(1)	29(1)	-2(1)	3(1)	3(1)
O(1)	31(1)	24(1)	39(1)	2(1)	1(1)	7(1)
N(1)	22(1)	18(1)	19(1)	1(1)	1(1)	2(1)
N(2)	24(1)	17(1)	20(1)	-1(1)	1(1)	1(1)
C(1)	23(1)	21(1)	21(1)	2(1)	1(1)	-3(1)
C(2)	20(1)	17(1)	20(1)	1(1)	3(1)	2(1)
C(3)	27(1)	25(1)	19(1)	-1(1)	0(1)	4(1)
C(4)	30(1)	24(1)	21(1)	-3(1)	-2(1)	2(1)
C(5)	25(1)	18(1)	29(1)	4(1)	3(1)	1(1)
C(6)	44(1)	32(1)	23(1)	3(1)	-3(1)	8(1)
C(7)	54(1)	28(1)	31(1)	-8(1)	-11(1)	-2(1)
C(8)	38(1)	17(1)	26(1)	1(1)	1(1)	-2(1)
C(9)	20(1)	21(1)	22(1)	0(1)	4(1)	-1(1)
C(10)	24(1)	22(1)	26(1)	-3(1)	6(1)	-1(1)
C(11)	32(1)	32(1)	26(1)	-9(1)	6(1)	-3(1)
C(12)	37(1)	42(1)	23(1)	-2(1)	6(1)	-2(1)
C(13)	40(1)	33(1)	26(1)	5(1)	9(1)	-4(1)

C(14)	29(1)	25(1)	25(1)	1(1)	5(1)	-5(1)
C(15)	19(1)	16(1)	29(1)	-1(1)	2(1)	-1(1)
C(16)	24(1)	26(1)	36(1)	3(1)	9(1)	2(1)
C(17)	24(1)	27(1)	54(1)	3(1)	10(1)	3(1)
C(18)	21(1)	26(1)	58(1)	-2(1)	-6(1)	2(1)
C(19)	30(1)	31(1)	36(1)	-4(1)	-8(1)	3(1)
C(20)	25(1)	28(1)	28(1)	-3(1)	0(1)	3(1)
C(21)	25(1)	17(1)	22(1)	-1(1)	2(1)	-3(1)
C(22)	27(1)	25(1)	32(1)	-6(1)	8(1)	-7(1)
C(23)	33(1)	28(1)	35(1)	-5(1)	5(1)	-13(1)
C(24)	42(1)	20(1)	39(1)	-8(1)	0(1)	-6(1)
C(25)	35(1)	23(1)	45(1)	-11(1)	3(1)	2(1)
C(26)	25(1)	21(1)	35(1)	-6(1)	3(1)	0(1)
C(27)	36(1)	20(1)	22(1)	1(1)	8(1)	2(1)
C(28)	44(1)	26(1)	27(1)	-4(1)	7(1)	-3(1)
C(29)	64(1)	26(1)	28(1)	-5(1)	8(1)	-2(1)
C(30)	77(2)	28(1)	30(1)	-3(1)	20(1)	12(1)
C(31)	55(1)	38(1)	39(1)	-1(1)	21(1)	16(1)
C(32)	39(1)	30(1)	32(1)	-1(1)	12(1)	6(1)
C(33)	23(1)	22(1)	22(1)	1(1)	5(1)	0(1)
C(34)	45(1)	29(1)	26(1)	0(1)	-4(1)	0(1)
C(35)	60(1)	42(1)	27(1)	5(1)	-10(1)	5(1)
C(36)	42(1)	34(1)	32(1)	11(1)	3(1)	7(1)
C(37)	42(1)	23(1)	32(1)	4(1)	8(1)	2(1)
C(38)	40(1)	23(1)	24(1)	0(1)	6(1)	1(1)
C(39)	20(1)	23(1)	28(1)	-3(1)	5(1)	0(1)
C(40)	25(1)	29(1)	46(1)	1(1)	7(1)	-4(1)
C(41)	25(1)	34(1)	77(2)	-10(1)	4(1)	-6(1)
C(42)	25(1)	44(1)	66(2)	-25(1)	-10(1)	9(1)
C(43)	31(1)	45(1)	39(1)	-6(1)	-5(1)	14(1)
C(44)	24(1)	29(1)	31(1)	0(1)	3(1)	6(1)
C(45)	44(3)	59(3)	25(2)	8(2)	-2(2)	-1(2)
C(46)	40(2)	77(4)	18(2)	7(2)	2(1)	21(2)
C(47)	110(5)	48(2)	23(2)	3(2)	5(2)	7(3)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for $Ru(IMe_4)(PPh_3)_2(CO)HF$ **(3)**.

Atom	x	y	z	U(eq)
H(5A)	3733	2350	5018	36
H(5B)	2885	2456	4555	36
H(5C)	3892	2335	4376	36
H(6A)	3039	1840	3489	50
H(6B)	2112	2015	3747	50
H(6C)	2149	1430	3386	50
H(7A)	2088	422	3574	58
H(7B)	1806	120	4127	58
H(7C)	2777	-29	3909	58
H(8A)	3511	168	5463	41
H(8B)	3539	-152	4879	41
H(8C)	2571	-9	5103	41
H(10)	5238	960	4695	29
H(11)	5145	937	3731	36
H(12)	5428	1786	3238	41

H(13)	5861	2651	3712	39
H(14)	5943	2679	4680	32
H(16)	7226	1481	5059	34
H(17)	8698	1194	5431	42
H(18)	9006	1015	6380	43
H(19)	7826	1108	6954	40
H(20)	6355	1400	6587	33
H(22)	7119	2603	5595	33
H(23)	7429	3550	5928	38
H(24)	6293	4087	6311	41
H(25)	4831	3679	6348	41
H(26)	4514	2727	6023	33
H(28)	4056	1940	7096	39
H(29)	3674	2634	7745	47
H(30)	2136	2789	7886	53
H(31)	983	2256	7378	52
H(32)	1355	1543	6748	40
H(34)	3753	912	7539	41
H(35)	4083	114	8124	53
H(36)	3808	-840	7801	43
H(37)	3273	-991	6872	39
H(38)	2983	-195	6276	34
H(40)	1500	240	6485	40
H(41)	143	35	5922	54
H(42)	-236	562	5108	55
H(43)	691	1348	4889	47
H(44)	2067	1549	5444	34
H(45)	780	682	7487	52
H(46)	1540	-180	7529	54
H(47)	893	-1072	7529	73
H(1)	4713	1494	6469	37(6)
H(45B)	0	-1309	7500	68
H(47A)	1406	-721	7514	83
H(46A)	1311	288	7552	92
H(45A)	0	772	7500	142

Table 11. Crystal data and structure refinement for $Ru(IEt_2Me_2)(PPh_3)_2(CO)HF$ **(4)**.

Compound	$Ru(IEt_2Me_2)(PPh_3)_2(CO)HF$ **(4)**
Empirical formula	C46 H47 F N2 O P2 Ru
Formula weight	825.87
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 23.5920(5)Å α = 90°
	b = 9.9650(2)Å β = 112.962(1)°
	c = 18.0880(5)Å γ = 90°
Volume	3915.44(16) $Å^3$
Z	4
Density (calculated)	1.401 Mg/m^3
Absorption coefficient	0.525 mm^{-1}
F(000)	1712
Crystal size	0.20 x 0.10 x 0.10 mm
Theta range for data collection	3.57 to 27.47°
Index ranges	-30<=h<=30; -12<=k<=12; -23<=l<=23
Reflections collected	23475
Independent reflections	4448 [R(int) = 0.0499]
Reflections observed (>2σ)	3874
Data Completeness	0.992
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.90 and 0.86
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4448 / 3 / 260
Goodness-of-fit on F^2	1.253
Final R indices [I>2σ(I)]	R^1 = 0.0428 wR_2 = 0.0917
R indices (all data)	R^1 = 0.0544 wR_2 = 0.0949
Largest diff. peak and hole	0.364 and -0.594 $eÅ^{-3}$

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IEt_2Me_2)(PPh_3)_2(CO)HF$ **(4)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	0	2169(1)	-2500	23(1)
P(1)	991(1)	2412(1)	-1487(1)	23(1)
N(1)	-372(1)	-889(2)	-2307(1)	23(1)
C(7)	1352(1)	823(3)	-1048(2)	27(1)
C(19)	1014(2)	3363(3)	-612(2)	30(1)
C(13)	1591(1)	3266(3)	-1723(2)	27(1)
C(2)	0	-35(4)	-2500	22(1)
C(4)	-859(1)	-510(3)	-2038(2)	29(1)
C(3)	-237(1)	-2238(3)	-2384(2)	29(1)
C(20)	1418(2)	3044(4)	165(2)	35(1)
C(8)	1010(2)	-19(3)	-762(2)	38(1)
C(16)	2517(2)	4488(4)	-2092(2)	46(1)
C(6)	-606(2)	-3375(3)	-2263(2)	43(1)
C(5)	-675(2)	-636(4)	-1138(2)	41(1)
C(12)	1904(2)	345(4)	-1056(2)	40(1)
C(21)	1444(2)	3829(4)	811(2)	47(1)

C(24)	641(2)	4480(4)	-725(2)	45(1)
C(18)	1974(2)	4215(4)	-1222(2)	46(1)
C(23)	670(2)	5264(4)	-74(3)	50(1)
C(22)	1066(2)	4933(4)	688(2)	50(1)
C(9)	1202(2)	-1307(4)	-517(2)	54(1)
C(14)	1684(2)	2932(4)	-2406(3)	57(1)
C(10)	1732(2)	-1787(4)	-559(2)	62(1)
C(17)	2430(2)	4823(5)	-1412(3)	59(1)
C(15)	2149(2)	3523(4)	-2587(3)	59(1)
C(11)	2090(2)	-965(5)	-820(2)	59(1)
C(1)	-300(15)	2380(30)	-1647(13)	21(3)
O(1)	-450(2)	2478(4)	-1145(3)	35(1)
F(1)	274(8)	2115(16)	-3402(8)	28(3)

Table 13. Bond lengths [Å] and angles [°] for $Ru(IEt_2Me_2)(PPh_3)_2(CO)HF$ **(4)**.

Ru(1)-H(1)	1.600(3)	Ru(1)-C(1)#1	1.944(5)
Ru(1)-C(1)	1.944(5)	Ru(1)-F(1)#1	1.976(5)
Ru(1)-F(1)	1.976(5)	Ru(1)-C(2)	2.196(4)
Ru(1)-P(1)	2.3540(7)	Ru(1)-P(1)#1	2.3540(7)
P(1)-C(7)	1.826(3)	P(1)-C(19)	1.827(3)
P(1)-C(13)	1.839(3)	N(1)-C(2)	1.361(3)
N(1)-C(3)	1.401(4)	N(1)-C(4)	1.463(4)
C(7)-C(12)	1.392(4)	C(7)-C(8)	1.396(5)
C(19)-C(24)	1.383(5)	C(19)-C(20)	1.393(4)
C(13)-C(18)	1.375(5)	C(13)-C(14)	1.377(5)
C(2)-N(1)#1	1.361(3)	C(4)-C(5)	1.517(4)
C(3)-C(3)#1	1.339(6)	C(3)-C(6)	1.497(4)
C(20)-C(21)	1.388(5)	C(8)-C(9)	1.376(5)
C(16)-C(17)	1.365(6)	C(16)-C(15)	1.369(6)
C(12)-C(11)	1.390(5)	C(21)-C(22)	1.379(6)
C(24)-C(23)	1.393(5)	C(18)-C(17)	1.390(5)
C(23)-C(22)	1.370(6)	C(9)-C(10)	1.369(6)
C(14)-C(15)	1.392(5)	C(10)-C(11)	1.384(7)
C(1)-O(1)	1.100(3)		
H(1)-Ru(1)-C(1)#1	83.7(10)	H(1)-Ru(1)-C(1)	83.7(10)
C(1)#1-Ru(1)-C(1)	167.4(19)	H(1)-Ru(1)-F(1)#1	91.6(5)
C(1)#1-Ru(1)-F(1)#1	174.7(8)	C(1)-Ru(1)-F(1)#1	8.2(14)
H(1)-Ru(1)-F(1)	91.6(5)	C(1)#1-Ru(1)-F(1)	8.2(14)
C(1)-Ru(1)-F(1)	174.7(8)	F(1)#1-Ru(1)-F(1)	176.9(9)
H(1)-Ru(1)-C(2)	180.0	C(1)#1-Ru(1)-C(2)	96.3(10)
C(1)-Ru(1)-C(2)	96.3(10)	F(1)#1-Ru(1)-C(2)	88.4(5)
F(1)-Ru(1)-C(2)	88.4(5)	H(1)-Ru(1)-P(1)	84.10(2)
C(1)#1-Ru(1)-P(1)	92.7(10)	C(1)-Ru(1)-P(1)	86.0(10)
F(1)#1-Ru(1)-P(1)	84.6(6)	F(1)-Ru(1)-P(1)	95.8(5)
C(2)-Ru(1)-P(1)	95.90(2)	H(1)-Ru(1)-P(1)#1	84.10(2)
C(1)#1-Ru(1)-P(1)#1	86.0(10)	C(1)-Ru(1)-P(1)#1	92.7(10)
F(1)#1-Ru(1)-P(1)#1	95.8(5)	F(1)-Ru(1)-P(1)#1	84.6(6)
C(2)-Ru(1)-P(1)#1	95.90(2)	P(1)-Ru(1)-P(1)#1	168.21(4)
C(7)-P(1)-C(19)	102.84(14)	C(7)-P(1)-C(13)	103.36(14)
C(19)-P(1)-C(13)	101.30(14)	C(7)-P(1)-Ru(1)	113.76(10)
C(19)-P(1)-Ru(1)	114.35(11)	C(13)-P(1)-Ru(1)	119.16(10)
C(2)-N(1)-C(3)	112.4(2)	C(2)-N(1)-C(4)	126.4(3)
C(3)-N(1)-C(4)	121.2(2)	C(12)-C(7)-C(8)	118.5(3)

C(12)-C(7)-P(1)	124.9(3)	C(8)-C(7)-P(1)	116.3(2)
C(24)-C(19)-C(20)	118.6(3)	C(24)-C(19)-P(1)	119.1(3)
C(20)-C(19)-P(1)	122.2(3)	C(18)-C(13)-C(14)	117.6(3)
C(18)-C(13)-P(1)	122.2(3)	C(14)-C(13)-P(1)	120.2(3)
N(1)#1-C(2)-N(1)	102.6(3)	N(1)#1-C(2)-Ru(1)	128.70(17)
N(1)-C(2)-Ru(1)	128.70(17)	N(1)-C(4)-C(5)	113.7(3)
C(3)#1-C(3)-N(1)	106.28(16)	C(3)#1-C(3)-C(6)	130.58(19)
N(1)-C(3)-C(6)	123.0(3)	C(21)-C(20)-C(19)	120.6(4)
C(9)-C(8)-C(7)	121.0(4)	C(17)-C(16)-C(15)	118.8(3)
C(11)-C(12)-C(7)	120.1(4)	C(22)-C(21)-C(20)	120.1(4)
C(19)-C(24)-C(23)	120.5(4)	C(13)-C(18)-C(17)	120.7(4)
C(22)-C(23)-C(24)	120.4(4)	C(23)-C(22)-C(21)	119.9(3)
C(10)-C(9)-C(8)	120.1(4)	C(13)-C(14)-C(15)	121.6(4)
C(9)-C(10)-C(11)	120.3(4)	C(16)-C(17)-C(18)	121.2(4)
C(16)-C(15)-C(14)	120.0(4)	C(10)-C(11)-C(12)	120.0(4)
O(1)-C(1)-Ru(1)	177(3)		

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z-1/2

Table 14. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IEt_2Me_2)(PPh_3)_2(CO)HF$ **(4)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	21(1)	18(1)	28(1)	0	7(1)	0
P(1)	22(1)	23(1)	25(1)	0(1)	9(1)	-1(1)
N(1)	25(1)	22(1)	25(1)	1(1)	11(1)	-1(1)
C(7)	27(2)	28(2)	23(2)	-1(1)	5(1)	2(1)
C(19)	30(2)	32(2)	29(2)	-6(1)	14(1)	-7(1)
C(13)	23(2)	29(2)	31(2)	3(1)	10(1)	0(1)
C(2)	21(2)	23(2)	21(2)	0	7(2)	0
C(4)	25(2)	32(2)	33(2)	-3(1)	15(1)	-3(1)
C(3)	31(2)	21(2)	32(2)	1(1)	11(1)	0(1)
C(20)	36(2)	40(2)	31(2)	-5(1)	15(1)	-10(2)
C(8)	38(2)	35(2)	35(2)	9(2)	5(2)	-4(2)
C(16)	28(2)	51(2)	58(2)	17(2)	18(2)	-5(2)
C(6)	40(2)	27(2)	62(2)	5(2)	23(2)	-5(2)
C(5)	40(2)	57(2)	33(2)	-1(2)	22(2)	-12(2)
C(12)	34(2)	55(2)	29(2)	4(2)	9(2)	16(2)
C(21)	54(2)	57(3)	33(2)	-12(2)	20(2)	-20(2)
C(24)	41(2)	45(2)	45(2)	-11(2)	12(2)	4(2)
C(18)	47(2)	52(2)	42(2)	-8(2)	21(2)	-22(2)
C(23)	47(2)	45(2)	66(3)	-25(2)	30(2)	-7(2)
C(22)	61(3)	56(3)	51(2)	-29(2)	39(2)	-30(2)
C(9)	58(3)	33(2)	49(2)	11(2)	-2(2)	-4(2)
C(14)	71(3)	58(3)	60(3)	-22(2)	46(2)	-37(2)
C(10)	87(3)	34(2)	38(2)	2(2)	-4(2)	20(2)
C(17)	55(3)	68(3)	51(2)	-8(2)	19(2)	-36(2)
C(15)	73(3)	58(3)	70(3)	-7(2)	55(3)	-17(2)
C(11)	64(3)	68(3)	37(2)	5(2)	11(2)	41(2)
C(1)	21(5)	13(8)	29(5)	-6(4)	10(4)	2(5)
O(1)	40(3)	36(3)	34(2)	-8(2)	20(2)	-5(2)
F(1)	30(4)	21(7)	32(3)	2(3)	12(3)	-2(4)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacementparameters ($Å^2$ x 10^3) for $Ru(IEt_2Me_2)(PPh_3)_2(CO)HF$ **(4)**.

Atom	x	y	z	U(eq)
H(4A)	-1223	-1086	-2314	35
H(4B)	-981	430	-2199	35
H(20)	1679	2283	254	42
H(8)	639	303	-736	46
H(16)	2827	4916	-2220	55
H(6A)	-455	-4224	-2391	64
H(6C)	-1040	-3258	-2618	64
H(6B)	-566	-3389	-1703	64
H(5A)	-500	-1528	-961	61
H(5C)	-1038	-510	-1009	61
H(5B)	-367	51	-863	61
H(12)	2155	915	-1223	48
H(21)	1722	3605	1339	56
H(24)	364	4715	-1251	54
H(18)	1925	4457	-742	55
H(23)	414	6033	-159	60
H(22)	1080	5464	1131	60
H(9)	966	-1864	-318	64
H(14)	1424	2283	-2763	68
H(10)	1855	-2688	-408	74
H(17)	2687	5483	-1061	70
H(15)	2211	3256	-3054	70
H(11)	2462	-1297	-838	71
H(1)	0	3774(3)	-2500	12(10)

Table 16. Crystal data and structure refinement for $Ru(ICy)(PPh_3)_2(CO)HF$ **(6)**.

Compound	$Ru(ICy)(PPh_3)_2(CO)HF$ **(6)**
Empirical formula	C52 H55 F N2 O P2 Ru
Formula weight	905.99
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/n
Unit cell dimensions	a = 9.1570(1)Å α = 90°
	b = 23.8970(4)Å β = 92.436(1)°
	c = 20.5620(3)Å γ = 90°
Volume	4495.41(11) $Å^3$
Z	4
Density (calculated)	1.339 Mg/m^3
Absorption coefficient	0.464 mm^{-1}
F(000)	1888
Crystal size	0.15 x 0.10 x 0.05 mm
Theta range for data collection	3.79 to 25.03°
Index ranges	-10<=h<=10; -25<=k<=28; -24<=l<=24
Reflections collected	35757
Independent reflections	7755 [R(int) = 0.0753]
Reflections observed (>2σ)	6130
Data Completeness	0.977
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.96 and 0.91
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7755 / 9 / 549
Goodness-of-fit on F^2	1.022
Final R indices [I>2σ(I)]	R1 = 0.0404 wR2 = 0.0792
R indices (all data)	R1 = 0.0600 wR2 = 0.0869
Largest diff. peak and hole	0.621 and -0.990 $eÅ^{-3}$

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(ICy)(PPh_3)_2(CO)HF$ **(6)**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	946(1)	2564(1)	-1345(1)	30(1)
P(2)	576(1)	3500(1)	-1037(1)	28(1)
P(3)	526(1)	1652(1)	-1737(1)	27(1)
C(1A)	680(30)	2720(20)	-2264(6)	30(9)
C(1)	856(13)	2385(5)	-472(3)	32(2)
O(1)	787(3)	2280(1)	93(1)	42(1)
O(1A)	561(13)	2797(6)	-2842(4)	60(3)
N(1)	4339(2)	2264(1)	-1006(1)	28(1)
N(2)	4197(2)	2878(1)	-1765(1)	27(1)
F(1A)	1130(20)	2418(11)	-456(6)	34(6)
C(2)	3336(3)	2569(1)	-1372(1)	27(1)
C(3)	5755(3)	2382(1)	-1171(2)	33(1)
C(4)	5663(3)	2765(1)	-1643(2)	34(1)
C(5)	4015(3)	1843(1)	-509(1)	32(1)
C(6)	4839(3)	1301(1)	-619(2)	34(1)
C(7)	4377(4)	860(2)	-139(2)	43(1)

C(8)	4706(5)	1055(2)	559(2)	55(1)
C(9)	3948(5)	1611(2)	680(2)	58(1)
C(10)	4344(4)	2056(2)	179(1)	43(1)
C(11)	3701(3)	3281(1)	-2271(1)	33(1)
C(12)	4555(3)	3825(1)	-2212(2)	38(1)
C(13)	3893(4)	4249(2)	-2694(2)	50(1)
C(14)	3924(5)	4026(2)	-3382(2)	61(1)
C(15)	3170(5)	3463(2)	-3449(2)	64(1)
C(16)	3784(4)	3036(2)	-2949(2)	47(1)
C(17)	2178(3)	3957(1)	-902(1)	32(1)
C(18)	2266(3)	4501(2)	-1136(2)	43(1)
C(19)	3514(4)	4821(2)	-1006(2)	53(1)
C(20)	4681(4)	4601(2)	-645(2)	53(1)
C(21)	4607(3)	4061(2)	-408(2)	46(1)
C(22)	3368(3)	3741(2)	-536(1)	36(1)
C(23)	-622(3)	3927(1)	-1577(1)	30(1)
C(24)	-700(4)	3808(2)	-2240(2)	47(1)
C(25)	-1550(4)	4138(2)	-2659(2)	56(1)
C(26)	-2316(4)	4585(2)	-2427(2)	48(1)
C(27)	-2267(4)	4702(2)	-1771(2)	47(1)
C(28)	-1427(4)	4367(2)	-1345(2)	42(1)
C(29)	-323(3)	3577(1)	-262(1)	32(1)
C(30)	72(4)	3982(2)	196(2)	40(1)
C(31)	-672(4)	4033(2)	772(2)	49(1)
C(32)	-1819(4)	3685(2)	890(2)	50(1)
C(33)	-2241(4)	3291(2)	443(2)	55(1)
C(34)	-1502(4)	3235(2)	-130(2)	48(1)
C(35)	-520(3)	1634(1)	-2519(1)	30(1)
C(36)	-1555(4)	2048(2)	-2663(2)	50(1)
C(37)	-2341(4)	2050(2)	-3254(2)	58(1)
C(38)	-2105(4)	1638(2)	-3713(2)	48(1)
C(39)	-1070(4)	1232(2)	-3579(2)	47(1)
C(40)	-280(4)	1227(2)	-2987(2)	40(1)
C(41)	-478(3)	1172(1)	-1229(1)	30(1)
C(42)	-1653(3)	853(2)	-1458(2)	41(1)
C(43)	-2326(4)	472(2)	-1063(2)	49(1)
C(44)	-1834(4)	398(2)	-430(2)	51(1)
C(45)	-670(4)	703(2)	-194(2)	65(1)
C(46)	-4(4)	1089(2)	-587(2)	55(1)
C(47)	2120(3)	1227(1)	-1932(1)	31(1)
C(48)	3184(3)	1493(2)	-2291(1)	37(1)
C(49)	4410(3)	1208(2)	-2482(2)	45(1)
C(50)	4581(4)	653(2)	-2321(2)	52(1)
C(51)	3561(4)	382(2)	-1968(2)	50(1)
C(52)	2313(3)	668(2)	-1772(2)	42(1)
F(1)	957(5)	2730(3)	-2309(1)	29(1)

Table 18. Bond lengths [Å] and angles [º] for $Ru(ICy)(PPh_3)_2(CO)HF$ **(6)**.

Ru(1)-H(1)	1.588(10)	Ru(1)-C(1)	1.851(5)
Ru(1)-F(1A)	1.863(12)	Ru(1)-C(1A)	1.930(8)
Ru(1)-F(1)	2.021(2)	Ru(1)-C(2)	2.192(3)
Ru(1)-P(3)	2.3497(8)	Ru(1)-P(2)	2.3534(8)
P(2)-C(29)	1.834(3)	P(2)-C(23)	1.836(3)
P(2)-C(17)	1.840(3)	P(3)-C(41)	1.825(3)

P(3)-C(47)	1.837(3)	P(3)-C(35)	1.838(3)
C(1A)-O(1A)	1.205(8)	C(1)-O(1)	1.194(6)
N(1)-C(2)	1.372(4)	N(1)-C(3)	1.384(4)
N(1)-C(5)	1.471(4)	N(2)-C(2)	1.370(4)
N(2)-C(4)	1.382(4)	N(2)-C(11)	1.475(4)
C(3)-C(4)	1.334(4)	C(5)-C(6)	1.520(4)
C(5)-C(10)	1.522(4)	C(6)-C(7)	1.517(4)
C(7)-C(8)	1.526(5)	C(8)-C(9)	1.525(5)
C(9)-C(10)	1.535(5)	C(11)-C(16)	1.517(4)
C(11)-C(12)	1.519(4)	C(12)-C(13)	1.524(4)
C(13)-C(14)	1.513(6)	C(14)-C(15)	1.516(6)
C(15)-C(16)	1.537(5)	C(17)-C(18)	1.390(5)
C(17)-C(22)	1.396(4)	C(18)-C(19)	1.391(5)
C(19)-C(20)	1.378(5)	C(20)-C(21)	1.383(6)
C(21)-C(22)	1.385(4)	C(23)-C(28)	1.380(4)
C(23)-C(24)	1.391(4)	C(24)-C(25)	1.383(5)
C(25)-C(26)	1.374(6)	C(26)-C(27)	1.378(5)
C(27)-C(28)	1.395(5)	C(29)-C(30)	1.387(4)
C(29)-C(34)	1.390(5)	C(30)-C(31)	1.397(5)
C(31)-C(32)	1.369(5)	C(32)-C(33)	1.359(5)
C(33)-C(34)	1.391(5)	C(35)-C(40)	1.392(4)
C(35)-C(36)	1.392(5)	C(36)-C(37)	1.386(4)
C(37)-C(38)	1.388(5)	C(38)-C(39)	1.377(5)
C(39)-C(40)	1.391(4)	C(41)-C(42)	1.384(4)
C(41)-C(46)	1.387(4)	C(42)-C(43)	1.383(5)
C(43)-C(44)	1.370(5)	C(44)-C(45)	1.363(5)
C(45)-C(46)	1.384(5)	C(47)-C(52)	1.384(5)
C(47)-C(48)	1.400(4)	C(48)-C(49)	1.385(4)
C(49)-C(50)	1.373(6)	C(50)-C(51)	1.370(5)
C(51)-C(52)	1.405(5)		
H(1)-Ru(1)-C(1)	88.2(11)	H(1)-Ru(1)-F(1A)	95.9(12)
C(1)-Ru(1)-F(1A)	8.3(9)	H(1)-Ru(1)-C(1A)	82.2(13)
C(1)-Ru(1)-C(1A)	170.0(10)	F(1A)-Ru(1)-C(1A)	178.1(9)
H(1)-Ru(1)-F(1)	89.7(10)	C(1)-Ru(1)-F(1)	176.9(4)
F(1A)-Ru(1)-F(1)	174.4(7)	C(1A)-Ru(1)-F(1)	7.4(9)
H(1)-Ru(1)-C(2)	174.9(10)	C(1)-Ru(1)-C(2)	96.4(4)
F(1A)-Ru(1)-C(2)	88.5(6)	C(1A)-Ru(1)-C(2)	93.3(8)
F(1)-Ru(1)-C(2)	85.87(15)	H(1)-Ru(1)-P(3)	83.4(11)
C(1)-Ru(1)-P(3)	96.0(3)	F(1A)-Ru(1)-P(3)	99.7(8)
C(1A)-Ru(1)-P(3)	80.3(17)	F(1)-Ru(1)-P(3)	81.6(2)
C(2)-Ru(1)-P(3)	98.35(8)	H(1)-Ru(1)-P(2)	78.9(11)
C(1)-Ru(1)-P(2)	86.9(3)	F(1A)-Ru(1)-P(2)	85.6(8)
C(1A)-Ru(1)-P(2)	93.9(17)	F(1)-Ru(1)-P(2)	94.8(2)
C(2)-Ru(1)-P(2)	99.03(8)	P(3)-Ru(1)-P(2)	161.94(3)
C(29)-P(2)-C(23)	101.00(13)	C(29)-P(2)-C(17)	101.17(14)
C(23)-P(2)-C(17)	102.40(14)	C(29)-P(2)-Ru(1)	113.84(11)
C(23)-P(2)-Ru(1)	117.04(10)	C(17)-P(2)-Ru(1)	118.74(10)
C(41)-P(3)-C(47)	101.64(14)	C(41)-P(3)-C(35)	103.27(13)
C(47)-P(3)-C(35)	100.65(13)	C(41)-P(3)-Ru(1)	117.77(10)
C(47)-P(3)-Ru(1)	117.93(10)	C(35)-P(3)-Ru(1)	113.15(11)
O(1A)-C(1A)-Ru(1)	177(4)	O(1)-C(1)-Ru(1)	178.7(9)
C(2)-N(1)-C(3)	111.7(2)	C(2)-N(1)-C(5)	126.4(2)
C(3)-N(1)-C(5)	121.9(2)	C(2)-N(2)-C(4)	111.5(2)
C(2)-N(2)-C(11)	126.9(2)	C(4)-N(2)-C(11)	121.6(2)

N(2)-C(2)-N(1)	102.8(2)	N(2)-C(2)-Ru(1)	128.17(19)
N(1)-C(2)-Ru(1)	129.0(2)	C(4)-C(3)-N(1)	106.7(3)
C(3)-C(4)-N(2)	107.3(3)	N(1)-C(5)-C(6)	111.3(2)
N(1)-C(5)-C(10)	112.3(3)	C(6)-C(5)-C(10)	110.0(3)
C(7)-C(6)-C(5)	110.0(3)	C(6)-C(7)-C(8)	110.4(3)
C(9)-C(8)-C(7)	110.3(3)	C(8)-C(9)-C(10)	111.8(3)
C(5)-C(10)-C(9)	110.4(3)	N(2)-C(11)-C(16)	111.7(3)
N(2)-C(11)-C(12)	111.1(2)	C(16)-C(11)-C(12)	111.0(3)
C(11)-C(12)-C(13)	109.1(3)	C(14)-C(13)-C(12)	110.5(3)
C(13)-C(14)-C(15)	111.8(3)	C(14)-C(15)-C(16)	112.0(3)
C(11)-C(16)-C(15)	109.1(3)	C(18)-C(17)-C(22)	118.5(3)
C(18)-C(17)-P(2)	124.0(2)	C(22)-C(17)-P(2)	117.5(2)
C(17)-C(18)-C(19)	120.4(3)	C(20)-C(19)-C(18)	120.4(4)
C(19)-C(20)-C(21)	119.8(3)	C(20)-C(21)-C(22)	120.0(3)
C(21)-C(22)-C(17)	120.8(3)	C(28)-C(23)-C(24)	119.2(3)
C(28)-C(23)-P(2)	121.9(2)	C(24)-C(23)-P(2)	118.9(2)
C(25)-C(24)-C(23)	119.9(3)	C(26)-C(25)-C(24)	120.6(3)
C(25)-C(26)-C(27)	120.1(3)	C(26)-C(27)-C(28)	119.5(3)
C(23)-C(28)-C(27)	120.6(3)	C(30)-C(29)-C(34)	117.4(3)
C(30)-C(29)-P(2)	123.1(2)	C(34)-C(29)-P(2)	119.4(2)
C(29)-C(30)-C(31)	120.9(3)	C(32)-C(31)-C(30)	120.2(3)
C(33)-C(32)-C(31)	120.0(3)	C(32)-C(33)-C(34)	120.3(4)
C(29)-C(34)-C(33)	121.3(3)	C(40)-C(35)-C(36)	118.4(3)
C(40)-C(35)-P(3)	122.0(2)	C(36)-C(35)-P(3)	119.6(2)
C(37)-C(36)-C(35)	120.9(3)	C(36)-C(37)-C(38)	120.2(4)
C(39)-C(38)-C(37)	119.4(3)	C(38)-C(39)-C(40)	120.6(3)
C(39)-C(40)-C(35)	120.5(3)	C(42)-C(41)-C(46)	116.9(3)
C(42)-C(41)-P(3)	123.7(2)	C(46)-C(41)-P(3)	119.3(2)
C(43)-C(42)-C(41)	121.5(3)	C(44)-C(43)-C(42)	120.3(3)
C(45)-C(44)-C(43)	119.3(3)	C(44)-C(45)-C(46)	120.4(3)
C(45)-C(46)-C(41)	121.6(3)	C(52)-C(47)-C(48)	118.6(3)
C(52)-C(47)-P(3)	125.2(2)	C(48)-C(47)-P(3)	116.2(3)
C(49)-C(48)-C(47)	121.1(3)	C(50)-C(49)-C(48)	119.5(3)
C(51)-C(50)-C(49)	120.7(3)	C(50)-C(51)-C(52)	120.2(4)
C(47)-C(52)-C(51)	119.9(3)		

Table 19. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(ICy)(PPh_3)_2(CO)HF$ **(6)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	25(1)	25(1)	41(1)	-5(1)	2(1)	-1(1)
P(2)	27(1)	26(1)	30(1)	-3(1)	1(1)	0(1)
P(3)	26(1)	27(1)	28(1)	-4(1)	3(1)	-2(1)
C(1)	27(4)	26(4)	42(4)	-13(2)	-1(2)	4(3)
O(1)	56(2)	45(2)	26(2)	6(1)	10(1)	12(1)
N(1)	26(1)	26(2)	31(1)	1(1)	-1(1)	-1(1)
N(2)	26(1)	24(2)	32(1)	0(1)	0(1)	1(1)
C(2)	30(1)	21(2)	29(2)	-5(1)	0(1)	1(1)
C(3)	26(1)	31(2)	44(2)	3(1)	-2(1)	-1(1)
C(4)	25(1)	34(2)	43(2)	3(2)	4(1)	1(1)
C(5)	38(2)	27(2)	29(2)	1(1)	-1(1)	-4(1)
C(6)	38(2)	28(2)	34(2)	1(1)	-4(1)	-2(1)
C(7)	51(2)	30(2)	46(2)	5(2)	0(2)	-1(2)

C(8)	83(3)	43(3)	39(2)	13(2)	2(2)	1(2)
C(9)	95(3)	50(3)	29(2)	4(2)	8(2)	2(2)
C(10)	62(2)	36(2)	32(2)	-3(2)	2(2)	-1(2)
C(11)	34(2)	29(2)	35(2)	7(1)	-1(1)	2(1)
C(12)	38(2)	31(2)	45(2)	8(2)	2(1)	-1(1)
C(13)	50(2)	41(2)	58(2)	22(2)	-1(2)	-1(2)
C(14)	68(2)	59(3)	57(2)	32(2)	2(2)	8(2)
C(15)	84(3)	69(3)	38(2)	12(2)	-9(2)	2(2)
C(16)	59(2)	48(2)	35(2)	5(2)	-1(2)	0(2)
C(17)	31(2)	31(2)	34(2)	-10(1)	1(1)	-1(1)
C(18)	36(2)	29(2)	63(2)	-5(2)	6(2)	0(1)
C(19)	44(2)	34(2)	80(3)	-11(2)	13(2)	-8(2)
C(20)	42(2)	53(3)	63(2)	-26(2)	11(2)	-17(2)
C(21)	32(2)	66(3)	39(2)	-18(2)	-1(1)	-2(2)
C(22)	35(2)	40(2)	32(2)	-7(1)	3(1)	-2(1)
C(23)	28(2)	29(2)	34(2)	3(1)	1(1)	-1(1)
C(24)	43(2)	63(3)	34(2)	2(2)	2(2)	11(2)
C(25)	52(2)	79(3)	38(2)	8(2)	0(2)	9(2)
C(26)	39(2)	55(3)	49(2)	25(2)	-6(2)	-5(2)
C(27)	40(2)	35(2)	65(2)	8(2)	4(2)	9(2)
C(28)	46(2)	41(2)	40(2)	0(2)	1(2)	12(2)
C(29)	31(2)	35(2)	29(2)	2(1)	-1(1)	5(1)
C(30)	41(2)	38(2)	39(2)	-5(2)	4(1)	3(2)
C(31)	54(2)	58(3)	34(2)	-12(2)	3(2)	12(2)
C(32)	45(2)	75(3)	32(2)	1(2)	7(2)	13(2)
C(33)	43(2)	78(3)	44(2)	-1(2)	13(2)	-11(2)
C(34)	44(2)	61(3)	38(2)	-7(2)	3(2)	-13(2)
C(35)	26(1)	37(2)	27(2)	-2(1)	3(1)	-6(1)
C(36)	42(2)	71(3)	37(2)	-11(2)	-1(2)	14(2)
C(37)	45(2)	82(3)	47(2)	1(2)	-9(2)	18(2)
C(38)	45(2)	67(3)	30(2)	1(2)	-6(2)	-10(2)
C(39)	61(2)	46(2)	34(2)	-9(2)	-2(2)	-12(2)
C(40)	49(2)	36(2)	35(2)	-4(2)	-3(1)	-4(2)
C(41)	29(2)	27(2)	33(2)	-2(1)	3(1)	-1(1)
C(42)	46(2)	45(2)	33(2)	-7(2)	6(1)	-15(2)
C(43)	53(2)	44(2)	51(2)	-7(2)	12(2)	-19(2)
C(44)	46(2)	45(2)	62(2)	18(2)	14(2)	-2(2)
C(45)	57(2)	92(4)	45(2)	26(2)	-7(2)	-21(2)
C(46)	48(2)	74(3)	42(2)	7(2)	-6(2)	-26(2)
C(47)	30(2)	32(2)	31(2)	-10(1)	-1(1)	-1(1)
C(48)	34(2)	45(2)	31(2)	-9(1)	2(1)	-1(1)
C(49)	34(2)	65(3)	37(2)	-17(2)	5(1)	4(2)
C(50)	35(2)	69(3)	52(2)	-30(2)	-2(2)	10(2)
C(51)	45(2)	33(2)	69(2)	-21(2)	-12(2)	10(2)
C(52)	37(2)	31(2)	56(2)	-16(2)	-3(2)	-2(2)
F(1)	31(2)	35(2)	21(2)	0(1)	4(1)	-2(2)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(ICy)(PPh_3)_2(CO)HF$ **(6)**.

Atom	x	y	z	U(eq)
H(3)	6625	2222	-984	40
H(4)	6458	2929	-1856	41
H(5)	2946	1758	-552	38
H(6A)	4632	1168	-1069	41
H(6B)	5904	1369	-561	41
H(7A)	4906	507	-217	51
H(7B)	3317	786	-204	51
H(8A)	4363	770	867	66
H(8B)	5775	1099	635	66
H(9A)	4235	1747	1122	69
H(9B)	2877	1554	660	69
H(10A)	3776	2401	252	52
H(10B)	5396	2149	234	52
H(11)	2653	3369	-2200	39
H(12A)	5592	3758	-2306	46
H(12B)	4515	3972	-1763	46
H(13A)	2871	4329	-2585	60
H(13B)	4452	4603	-2661	60
H(14A)	4951	3988	-3506	74
H(14B)	3434	4296	-3683	74
H(15A)	3295	3316	-3894	77
H(15B)	2110	3512	-3390	77
H(16A)	3211	2685	-2981	56
H(16B)	4813	2948	-3040	56
H(18)	1468	4655	-1386	51
H(19)	3562	5192	-1167	63
H(20)	5533	4821	-559	63
H(21)	5407	3910	-156	55
H(22)	3326	3369	-373	43
H(24)	-169	3501	-2404	56
H(25)	-1606	4054	-3111	67
H(26)	-2880	4814	-2720	57
H(27)	-2801	5010	-1609	56
H(28)	-1410	4441	-890	51
H(30)	860	4228	117	47
H(31)	-381	4309	1084	58
H(32)	-2320	3719	1283	60
H(33)	-3045	3053	523	66
H(34)	-1808	2958	-438	57
H(36)	-1724	2332	-2352	60
H(37)	-3043	2336	-3345	70
H(38)	-2652	1636	-4116	57
H(39)	-895	952	-3894	57
H(40)	429	943	-2900	48
H(42)	-2005	898	-1896	49
H(43)	-3135	260	-1231	59
H(44)	-2299	137	-158	61
H(45)	-314	651	242	78
H(46)	797	1301	-412	66
H(48)	3063	1876	-2405	44

H(49)	5128	1394	-2722	54
H(50)	5415	455	-2456	63
H(51)	3698	-1	-1856	59
H(52)	1602	478	-1531	50
H(1)	-787(11)	2598(12)	-1378(13)	31(8)

Table 21. Crystal data and structure refinement for $Ru(IMe_4)(PPh_3)(CO)_3$ **(15)**.

Compound	$Ru(IMe_4)(PPh_3)(CO)_3$ **(15)**
Empirical formula	C34 H33 N2 O3 P Ru
Formula weight	649.66
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 17.0730(2)Å α = 90°
	b = 9.88300(1)Å β = 98.492(1)°
	c = 18.2210(2)Å γ = 90°
Volume	3040.77(6) $Å^3$
Z	4
Density (calculated)	1.419 Mg/m^3
Absorption coefficient	0.605 mm^{-1}
F(000)	1336
Crystal size	0.30 x 0.15 x 0.15 mm
Theta range for data collection	3.54 to 30.03°
Index ranges	-24<=h<=24; -13<=k<=13; -25<=l<=25
Reflections collected	65323
Independent reflections	8865 [R(int) = 0.0458]
Reflections observed (>2σ)	7025
Data Completeness	0.998
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.89 and 0.85
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8865 / 0 / 357
Goodness-of-fit on F^2	1.053
Final R indices [I>2σ(I)]	R^1 = 0.0330 wR_2 = 0.0718
R indices (all data)	R^1 = 0.0494 wR_2 = 0.0787
Largest diff. peak and hole	0.737 and -0.885 $eÅ^{-3}$

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IMe_4)(PPh_3)(CO)_3$ **(15)**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	-576(1)	2547(1)	7188(1)	21(1)
P(1)	129(1)	586(1)	7589(1)	22(1)
O(1)	-2029(1)	878(2)	6592(1)	45(1)
O(2)	667(1)	3348(2)	6210(1)	44(1)
O(3)	-453(1)	3229(2)	8847(1)	52(1)
N(1)	-1492(1)	5360(2)	7040(1)	26(1)
N(2)	-1565(1)	4370(2)	5989(1)	27(1)
C(1)	-1478(1)	1482(2)	6818(1)	29(1)
C(2)	216(1)	3049(2)	6595(1)	28(1)
C(3)	-508(1)	3056(2)	8217(1)	33(1)

C(4)	-1253(1)	4222(2)	6720(1)	23(1)
C(5)	-1276(1)	5710(2)	7823(1)	35(1)
C(6)	-1940(1)	6202(2)	6527(1)	30(1)
C(7)	-2248(2)	7547(2)	6718(1)	41(1)
C(8)	-1988(1)	5580(2)	5865(1)	30(1)
C(9)	-2384(2)	5983(3)	5109(1)	44(1)
C(10)	-1478(1)	3431(2)	5391(1)	37(1)
C(11)	1200(1)	774(2)	7855(1)	25(1)
C(12)	1489(1)	1980(2)	8188(1)	33(1)
C(13)	2295(1)	2137(2)	8445(1)	37(1)
C(14)	2815(1)	1098(2)	8369(1)	37(1)
C(15)	2540(1)	-100(2)	8033(1)	37(1)
C(16)	1737(1)	-262(2)	7774(1)	32(1)
C(17)	-164(1)	-269(2)	8402(1)	25(1)
C(18)	383(1)	-833(2)	8961(1)	36(1)
C(19)	130(2)	-1552(3)	9541(1)	44(1)
C(20)	-666(2)	-1719(2)	9567(1)	40(1)
C(21)	-1217(1)	-1159(2)	9016(1)	38(1)
C(22)	-968(1)	-425(2)	8441(1)	32(1)
C(23)	42(1)	-806(2)	6912(1)	24(1)
C(24)	123(1)	-2157(2)	7136(1)	30(1)
C(25)	61(1)	-3198(2)	6618(1)	35(1)
C(26)	-93(1)	-2905(2)	5871(1)	39(1)
C(27)	-177(2)	-1582(3)	5643(1)	44(1)
C(28)	-110(1)	-530(2)	6156(1)	35(1)
C(29)	2659(3)	1145(4)	6312(2)	44(1)
C(30)	2056(3)	805(5)	5764(3)	48(1)
C(31)	2240(5)	188(7)	5143(3)	49(2)
C(32)	2992(4)	-73(7)	5056(4)	50(2)
C(33)	3609(4)	235(6)	5608(3)	61(1)
C(34)	3435(4)	856(5)	6255(3)	52(1)
C(29A)	3042(3)	1080(5)	6345(2)	34(1)
C(30A)	2341(3)	893(6)	5861(3)	46(2)
C(31A)	2356(3)	293(7)	5173(3)	52(4)
C(32A)	3071(3)	-119(7)	4969(2)	42(3)
C(33A)	3772(3)	69(6)	5452(3)	49(2)
C(34A)	3757(3)	668(5)	6140(2)	47(2)

Table 23. Bond lengths [Å] and angles [°] for $Ru(IMe_4)(PPh_3)(CO)_3$ **(15)**.

Ru(1)-C(1)	1.904(2)	Ru(1)-C(2)	1.916(2)
Ru(1)-C(3)	1.929(2)	Ru(1)-C(4)	2.1239(18)
Ru(1)-P(1)	2.3408(5)	P(1)-C(11)	1.8304(19)
P(1)-C(17)	1.8377(19)	P(1)-C(23)	1.8397(19)
O(1)-C(1)	1.140(2)	O(2)-C(2)	1.154(2)
O(3)-C(3)	1.149(2)	N(1)-C(4)	1.358(2)
N(1)-C(6)	1.393(2)	N(1)-C(5)	1.461(3)
N(2)-C(4)	1.367(2)	N(2)-C(8)	1.398(2)
N(2)-C(10)	1.455(3)	C(6)-C(8)	1.346(3)
C(6)-C(7)	1.491(3)	C(8)-C(9)	1.496(3)
C(11)-C(12)	1.395(3)	C(11)-C(16)	1.397(3)
C(12)-C(13)	1.395(3)	C(13)-C(14)	1.379(3)
C(14)-C(15)	1.383(3)	C(15)-C(16)	1.392(3)
C(17)-C(18)	1.392(3)	C(17)-C(22)	1.393(3)
C(18)-C(19)	1.394(3)	C(19)-C(20)	1.377(3)

C(20)-C(21)	1.385(3)	C(21)-C(22)	1.391(3)
C(23)-C(28)	1.392(3)	C(23)-C(24)	1.397(3)
C(24)-C(25)	1.390(3)	C(25)-C(26)	1.378(3)
C(26)-C(27)	1.373(4)	C(27)-C(28)	1.391(3)
C(29)-C(30)	1.365(7)	C(29)-C(34)	1.373(7)
C(30)-C(31)	1.363(6)	C(31)-C(32)	1.341(8)
C(32)-C(33)	1.379(7)	C(33)-C(34)	1.400(8)
C(29A)-C(30A)	1.3900	C(29A)-C(34A)	1.3900
C(30A)-C(31A)	1.3900	C(31A)-C(32A)	1.3900
C(32A)-C(33A)	1.3900	C(33A)-C(34A)	1.3900
C(1)-Ru(1)-C(2)	123.05(9)	C(1)-Ru(1)-C(3)	114.65(9)
C(2)-Ru(1)-C(3)	122.29(9)	C(1)-Ru(1)-C(4)	85.70(8)
C(2)-Ru(1)-C(4)	87.71(7)	C(3)-Ru(1)-C(4)	97.94(8)
C(1)-Ru(1)-P(1)	90.24(6)	C(2)-Ru(1)-P(1)	91.00(6)
C(3)-Ru(1)-P(1)	87.56(6)	C(4)-Ru(1)-P(1)	174.16(5)
C(11)-P(1)-C(17)	102.35(8)	C(11)-P(1)-C(23)	103.40(8)
C(17)-P(1)-C(23)	101.03(9)	C(11)-P(1)-Ru(1)	116.49(6)
C(17)-P(1)-Ru(1)	116.39(6)	C(23)-P(1)-Ru(1)	115.02(6)
C(4)-N(1)-C(6)	112.06(16)	C(4)-N(1)-C(5)	124.59(16)
C(6)-N(1)-C(5)	123.27(16)	C(4)-N(2)-C(8)	111.50(16)
C(4)-N(2)-C(10)	126.37(16)	C(8)-N(2)-C(10)	122.13(17)
O(1)-C(1)-Ru(1)	177.99(18)	O(2)-C(2)-Ru(1)	176.77(18)
O(3)-C(3)-Ru(1)	173.33(19)	N(1)-C(4)-N(2)	103.42(15)
N(1)-C(4)-Ru(1)	130.77(13)	N(2)-C(4)-Ru(1)	125.80(13)
C(8)-C(6)-N(1)	106.52(17)	C(8)-C(6)-C(7)	129.80(19)
N(1)-C(6)-C(7)	123.62(19)	C(6)-C(8)-N(2)	106.50(17)
C(6)-C(8)-C(9)	131.56(19)	N(2)-C(8)-C(9)	121.94(19)
C(12)-C(11)-C(16)	118.47(18)	C(12)-C(11)-P(1)	118.54(15)
C(16)-C(11)-P(1)	122.91(15)	C(13)-C(12)-C(11)	120.7(2)
C(14)-C(13)-C(12)	120.1(2)	C(13)-C(14)-C(15)	120.1(2)
C(14)-C(15)-C(16)	120.1(2)	C(15)-C(16)-C(11)	120.6(2)
C(18)-C(17)-C(22)	118.56(18)	C(18)-C(17)-P(1)	122.71(15)
C(22)-C(17)-P(1)	118.63(15)	C(17)-C(18)-C(19)	120.6(2)
C(20)-C(19)-C(18)	120.3(2)	C(19)-C(20)-C(21)	119.7(2)
C(20)-C(21)-C(22)	120.2(2)	C(21)-C(22)-C(17)	120.6(2)
C(28)-C(23)-C(24)	118.24(18)	C(28)-C(23)-P(1)	120.13(15)
C(24)-C(23)-P(1)	121.63(15)	C(25)-C(24)-C(23)	121.0(2)
C(26)-C(25)-C(24)	120.0(2)	C(27)-C(26)-C(25)	119.6(2)
C(26)-C(27)-C(28)	120.9(2)	C(27)-C(28)-C(23)	120.2(2)
C(30)-C(29)-C(34)	121.7(4)	C(31)-C(30)-C(29)	118.4(5)
C(32)-C(31)-C(30)	121.7(7)	C(31)-C(32)-C(33)	120.9(7)
C(32)-C(33)-C(34)	118.4(6)	C(29)-C(34)-C(33)	118.8(5)
C(30A)-C(29A)-C(34A)	120.0	C(31A)-C(30A)-C(29A)	120.0
C(30A)-C(31A)-C(32A)	120.0	C(31A)-C(32A)-C(33A)	120.0
C(34A)-C(33A)-C(32A)	120.0	C(33A)-C(34A)-C(29A)	120.0

Table 24. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IMe_4)(PPh_3)(CO)_3$ **(15)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	22(1)	20(1)	22(1)	1(1)	1(1)	3(1)
P(1)	22(1)	20(1)	23(1)	1(1)	2(1)	1(1)
O(1)	37(1)	45(1)	50(1)	-2(1)	-2(1)	-8(1)
O(2)	41(1)	45(1)	50(1)	2(1)	18(1)	-4(1)
O(3)	81(1)	46(1)	27(1)	0(1)	4(1)	17(1)
N(1)	27(1)	22(1)	30(1)	3(1)	5(1)	4(1)
N(2)	28(1)	25(1)	28(1)	3(1)	1(1)	2(1)
C(1)	32(1)	26(1)	29(1)	2(1)	1(1)	5(1)
C(2)	28(1)	23(1)	34(1)	1(1)	3(1)	3(1)
C(3)	41(1)	27(1)	30(1)	1(1)	2(1)	10(1)
C(4)	22(1)	22(1)	26(1)	3(1)	2(1)	1(1)
C(5)	46(1)	28(1)	32(1)	-3(1)	8(1)	8(1)
C(6)	25(1)	24(1)	39(1)	8(1)	6(1)	4(1)
C(7)	45(1)	30(1)	49(1)	9(1)	14(1)	13(1)
C(8)	26(1)	27(1)	36(1)	11(1)	1(1)	3(1)
C(9)	47(1)	41(1)	42(1)	15(1)	-4(1)	8(1)
C(10)	47(1)	36(1)	26(1)	0(1)	-2(1)	6(1)
C(11)	25(1)	25(1)	23(1)	3(1)	-1(1)	1(1)
C(12)	32(1)	30(1)	36(1)	0(1)	2(1)	2(1)
C(13)	36(1)	38(1)	35(1)	-3(1)	-5(1)	-9(1)
C(14)	25(1)	54(1)	30(1)	4(1)	-2(1)	-5(1)
C(15)	25(1)	43(1)	42(1)	2(1)	3(1)	7(1)
C(16)	27(1)	32(1)	36(1)	-2(1)	1(1)	2(1)
C(17)	30(1)	21(1)	25(1)	1(1)	4(1)	2(1)
C(18)	32(1)	44(1)	30(1)	10(1)	3(1)	3(1)
C(19)	49(1)	52(2)	32(1)	15(1)	5(1)	5(1)
C(20)	55(1)	36(1)	32(1)	7(1)	17(1)	1(1)
C(21)	38(1)	35(1)	43(1)	5(1)	17(1)	0(1)
C(22)	32(1)	32(1)	34(1)	5(1)	7(1)	3(1)
C(23)	20(1)	23(1)	29(1)	-3(1)	2(1)	1(1)
C(24)	29(1)	27(1)	36(1)	0(1)	6(1)	0(1)
C(25)	30(1)	26(1)	52(1)	-6(1)	12(1)	-3(1)
C(26)	32(1)	38(1)	49(1)	-20(1)	11(1)	-4(1)
C(27)	53(1)	47(1)	32(1)	-10(1)	7(1)	2(1)
C(28)	45(1)	29(1)	31(1)	-1(1)	6(1)	4(1)

Table 25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IMe_4)(PPh_3)(CO)_3$ **(15)**.

Atom	x	y	z	U(eq)
H(5A)	-1559	5115	8126	53
H(5B)	-1421	6653	7901	53
H(5C)	-704	5596	7968	53
H(7A)	-2546	7957	6272	61
H(7B)	-1804	8136	6913	61
H(7C)	-2598	7433	7095	61
H(9A)	-2680	6824	5144	66
H(9B)	-2749	5266	4904	66
H(9C)	-1983	6122	4783	66
H(10A)	-1097	2724	5576	55
H(10B)	-1286	3921	4984	55
H(10C)	-1991	3017	5209	55
H(12)	1134	2702	8241	39
H(13)	2486	2962	8673	45
H(14)	3363	1204	8547	44
H(15)	2899	-815	7979	44
H(16)	1552	-1084	7539	38
H(18)	933	-726	8947	43
H(19)	509	-1928	9920	53
H(20)	-837	-2216	9960	48
H(21)	-1767	-1277	9030	45
H(22)	-1349	-27	8072	39
H(24)	222	-2367	7651	36
H(25)	125	-4111	6779	42
H(26)	-141	-3615	5516	47
H(27)	-282	-1382	5128	52
H(28)	-169	380	5989	42
H(29)	2539	1593	6743	52
H(30)	1522	994	5815	58
H(31)	1825	-65	4761	59
H(32)	3100	-475	4608	61
H(33)	4140	30	5550	73
H(34)	3846	1074	6647	62
H(29A)	3031	1490	6815	41
H(30A)	1851	1174	6000	55
H(31A)	1876	165	4842	63
H(32A)	3082	-528	4499	50
H(33A)	4262	-213	5313	59
H(34A)	4237	796	6471	56

Table 26. Crystal data and structure refinement for Ru(SIMes)(PPh_3)(CO)HF **(27)**.

Compound	Ru(SIMes)(PPh_3)(CO)HF **(27)**.
Empirical formula	C44 H48 F N2 O2 P Ru
Formula weight	787.88
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/a$
Unit cell dimensions	a = 13.7310(1)Å α = 90°
	b = 13.6060(1)Å β = 105.746(4)°
	c = 21.7640(3)Å γ = 90°
Volume	3913.46(7) $Å^3$
Z	4
Density (calculated)	1.337 Mg/m^3
Absorption coefficient	0.485 mm^{-1}
F(000)	1640
Crystal size	0.25 x 0.25 x 0.10 mm
Theta range for data collection	4.77 to 30.04°
Index ranges	-19<=h<=19; -19<=k<=19; -30<=l<=30
Reflections collected	79321
Independent reflections	11386 [R(int) = 0.0600]
Reflections observed (>2σ)	8514
Data Completeness	0.993
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.95 and 0.89
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11386 / 3 / 493
Goodness-of-fit on F^2	1.054
Final R indices [I>2σ(I)]	R1 = 0.0396 wR2 = 0.0945
R indices (all data)	R1 = 0.0646 wR2 = 0.1059
Largest diff. peak and hole	0.741 and -0.561 $eÅ^{-3}$

Table 26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIMes)(PPh_3)(CO)HF **(27)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	X	y	z	U(eq)
Ru(1)	4296(1)	-260(1)	7699(1)	24(1)
P(1)	5740(1)	733(1)	7911(1)	25(1)
F(1)	5190(1)	-1353(1)	7521(1)	41(1)
O(1)	3011(2)	1267(2)	8068(2)	50(1)
0(2)	3805(5)	2566(4)	5433(2)	124(2)
N(1)	2284(1)	-1418(2)	7093(1)	30(1)
N(2)	3006(1)	-1908(1)	8040(1)	29(1)
C(1)	3533(3)	678(3)	7944(2)	32(1)
C(2)	3114(2)	-1255(2)	7590(1)	28(1)
C(3)	1679(2)	-2160(2)	7234(1)	37(1)
C(4)	2130(2)	-2467(2)	7826(1)	36(1)
C(5)	2069(2)	-891(2)	6498(1)	33(1)
C(6)	1337(2)	-156(2)	6382(1)	42(1)
C(7)	1150(2)	340(2)	5805(1)	52(1)
C(8)	1668(3)	123(3)	5355(1)	53(1)
C(9)	2385(2)	-614(2)	5491(1)	48(1)

C(10)	2609(2)	-1139(2)	6059(1)	40(1)
C(11)	776(2)	107(3)	6864(1)	54(1)
C(12)	1449(3)	686(4)	4731(2)	82(1)
C(13)	3399(2)	-1941(2)	6203(2)	52(1)
C(14)	3716(2)	-1997(2)	8661(1)	30(1)
C(15)	4519(2)	-2653(2)	8737(1)	39(1)
C(16)	5194(2)	-2717(2)	9343(2)	46(1)
C(17)	5083(2)	-2165(2)	9852(1)	47(1)
C(18)	4265(2)	-1526(2)	9758(1)	43(1)
C(19)	3564(2)	-1437(2)	9163(1)	34(1)
C(20)	4638(2)	-3253(2)	8182(2)	49(1)
C(21)	5835(2)	-2240(3)	10507(2)	69(1)
C(22)	2683(2)	-748(2)	9075(1)	44(1)
C(23)	6746(2)	204(2)	8557(1)	27(1)
C(24)	6501(2)	-509(2)	8950(1)	35(1)
C(25)	7253(2)	-954(2)	9426(1)	42(1)
C(26)	8251(2)	-700(2)	9518(1)	43(1)
C(27)	8507(2)	10(2)	9138(2)	48(1)
C(28)	7760(2)	454(2)	8654(1)	38(1)
C(29)	5623(2)	2000(2)	8158(1)	26(1)
C(30)	6304(2)	2435(2)	8676(1)	32(1)
C(31)	6212(2)	3422(2)	8812(1)	39(1)
C(32)	5446(2)	3977(2)	8436(1)	41(1)
C(33)	4746(2)	3553(2)	7923(1)	38(1)
C(34)	4837(2)	2564(2)	7782(1)	31(1)
C(35)	6407(2)	896(2)	7292(1)	30(1)
C(36)	6722(2)	1804(2)	7130(1)	36(1)
C(37)	7254(2)	1869(2)	6668(1)	46(1)
C(38)	7482(2)	1039(3)	6380(1)	54(1)
C(39)	7188(3)	127(3)	6550(2)	62(1)
C(40)	6638(2)	56(2)	6995(2)	49(1)
C(41)	4134(6)	1846(7)	5879(3)	84(2)
C(42)	4647(5)	1069(5)	5592(3)	71(2)
C(43)	4992(5)	1638(6)	5093(3)	80(2)
C(44)	4159(5)	2372(5)	4883(3)	80(2)
O(1A)	2785(7)	1282(7)	7634(5)	74(3)
O(2A)	3896(11)	967(11)	5001(7)	126(4)
C(1A)	3399(8)	674(8)	7667(5)	41(3)
C(41A)	4050(20)	1346(18)	5671(11)	108(7)
C(42A)	4455(12)	2355(12)	5651(8)	73(4)
C(43A)	4872(14)	2323(13)	5098(8)	75(4)
C(44A)	4453(16)	1527(14)	4725(9)	92(5)

Table 27. Bond lengths [Å] and angles [°] for Ru(SIMes)(PPh_3)(CO)HF **(27)**.

Ru(1)-H(1)	1.602(10)	Ru(1)-C(1A)	1.758(9)
Ru(1)-C(1)	1.820(3)	Ru(1)-F(1)	2.0315(13)
Ru(1)-C(2)	2.077(2)	Ru(1)-P(1)	2.3403(6)
P(1)-C(29)	1.825(2)	P(1)-C(23)	1.830(2)
P(1)-C(35)	1.838(2)	O(1)-C(1)	1.155(4)
0(2)-C(41)	1.367(8)	0(2)-C(44)	1.433(7)
N(1)-C(2)	1.360(3)	N(1)-C(3)	1.394(3)
N(1)-C(5)	1.438(3)	N(2)-C(2)	1.359(3)
N(2)-C(4)	1.392(3)	N(2)-C(14)	1.440(3)
C(3)-C(4)	1.336(4)	C(5)-C(6)	1.391(4)

C(5)-C(10)	1.401(3)	C(6)-C(7)	1.388(4)
C(6)-C(11)	1.503(4)	C(7)-C(8)	1.390(4)
C(8)-C(9)	1.380(5)	C(8)-C(12)	1.517(4)
C(9)-C(10)	1.389(4)	C(10)-C(13)	1.510(4)
C(14)-C(15)	1.394(3)	C(14)-C(19)	1.395(4)
C(15)-C(16)	1.393(4)	C(15)-C(20)	1.504(4)
C(16)-C(17)	1.379(5)	C(17)-C(18)	1.391(4)
C(17)-C(21)	1.521(4)	C(18)-C(19)	1.394(4)
C(19)-C(22)	1.500(4)	C(23)-C(28)	1.392(3)
C(23)-C(24)	1.394(3)	C(24)-C(25)	1.387(4)
C(25)-C(26)	1.375(4)	C(26)-C(27)	1.378(4)
C(27)-C(28)	1.394(4)	C(29)-C(30)	1.387(3)
C(29)-C(34)	1.395(3)	C(30)-C(31)	1.388(3)
C(31)-C(32)	1.371(4)	C(32)-C(33)	1.386(4)
C(33)-C(34)	1.393(3)	C(35)-C(36)	1.385(3)
C(35)-C(40)	1.391(4)	C(36)-C(37)	1.397(4)
C(37)-C(38)	1.370(5)	C(38)-C(39)	1.385(5)
C(39)-C(40)	1.384(4)	C(41)-C(42)	1.496(9)
C(42)-C(43)	1.511(8)	C(43)-C(44)	1.493(8)
O(1A)-C(1A)	1.170(11)	O(2A)-C(44A)	1.33(2)
O(2A)-C(41A)	1.51(3)	C(41A)-C(42A)	1.49(3)
C(42A)-C(43A)	1.47(2)	C(43A)-C(44A)	1.38(2)
H(1)-Ru(1)-C(1A)	65.7(18)	H(1)-Ru(1)-C(1)	83.6(17)
C(1A)-Ru(1)-C(1)	18.6(3)	H(1)-Ru(1)-F(1)	102.2(17)
C(1A)-Ru(1)-F(1)	167.1(4)	C(1)-Ru(1)-F(1)	174.13(16)
H(1)-Ru(1)-C(2)	96.3(17)	C(1A)-Ru(1)-C(2)	87.1(4)
C(1)-Ru(1)-C(2)	89.82(13)	F(1)-Ru(1)-C(2)	89.71(7)
H(1)-Ru(1)-P(1)	89.9(17)	C(1A)-Ru(1)-P(1)	97.9(4)
C(1)-Ru(1)-P(1)	93.53(11)	F(1)-Ru(1)-P(1)	86.36(4)
C(2)-Ru(1)-P(1)	173.28(6)	C(29)-P(1)-C(23)	104.70(10)
C(29)-P(1)-C(35)	101.76(10)	C(23)-P(1)-C(35)	100.87(10)
C(29)-P(1)-Ru(1)	117.73(7)	C(23)-P(1)-Ru(1)	110.29(7)
C(35)-P(1)-Ru(1)	119.32(8)	C(41)-0(2)-C(44)	109.8(5)
C(2)-N(1)-C(3)	111.3(2)	C(2)-N(1)-C(5)	123.92(19)
C(3)-N(1)-C(5)	124.8(2)	C(2)-N(2)-C(4)	111.7(2)
C(2)-N(2)-C(14)	123.55(18)	C(4)-N(2)-C(14)	124.8(2)
O(1)-C(1)-Ru(1)	176.3(4)	N(2)-C(2)-N(1)	103.61(18)
N(2)-C(2)-Ru(1)	125.30(16)	N(1)-C(2)-Ru(1)	131.09(17)
C(4)-C(3)-N(1)	106.9(2)	C(3)-C(4)-N(2)	106.5(2)
C(6)-C(5)-C(10)	122.6(2)	C(6)-C(5)-N(1)	118.9(2)
C(10)-C(5)-N(1)	118.5(2)	C(7)-C(6)-C(5)	117.5(3)
C(7)-C(6)-C(11)	120.7(3)	C(5)-C(6)-C(11)	121.8(2)
C(6)-C(7)-C(8)	122.0(3)	C(9)-C(8)-C(7)	118.4(3)
C(9)-C(8)-C(12)	121.0(3)	C(7)-C(8)-C(12)	120.5(3)
C(8)-C(9)-C(10)	122.5(3)	C(9)-C(10)-C(5)	117.0(3)
C(9)-C(10)-C(13)	122.0(2)	C(5)-C(10)-C(13)	121.0(2)
C(15)-C(14)-C(19)	122.6(2)	C(15)-C(14)-N(2)	118.6(2)
C(19)-C(14)-N(2)	118.8(2)	C(16)-C(15)-C(14)	117.1(3)
C(16)-C(15)-C(20)	122.5(2)	C(14)-C(15)-C(20)	120.4(3)
C(17)-C(16)-C(15)	122.4(2)	C(16)-C(17)-C(18)	118.9(3)
C(16)-C(17)-C(21)	121.4(3)	C(18)-C(17)-C(21)	119.6(3)
C(17)-C(18)-C(19)	121.1(3)	C(18)-C(19)-C(14)	117.9(2)
C(18)-C(19)-C(22)	120.2(2)	C(14)-C(19)-C(22)	121.9(2)
C(28)-C(23)-C(24)	118.4(2)	C(28)-C(23)-P(1)	122.35(18)

C(24)-C(23)-P(1)	119.19(17)	C(25)-C(24)-C(23)	120.5(2)
C(26)-C(25)-C(24)	120.7(2)	C(25)-C(26)-C(27)	119.7(2)
C(26)-C(27)-C(28)	120.2(3)	C(23)-C(28)-C(27)	120.6(2)
C(30)-C(29)-C(34)	119.0(2)	C(30)-C(29)-P(1)	123.26(17)
C(34)-C(29)-P(1)	117.62(17)	C(29)-C(30)-C(31)	120.4(2)
C(32)-C(31)-C(30)	120.5(2)	C(31)-C(32)-C(33)	120.2(2)
C(32)-C(33)-C(34)	119.7(2)	C(33)-C(34)-C(29)	120.3(2)
C(36)-C(35)-C(40)	119.3(2)	C(36)-C(35)-P(1)	123.05(19)
C(40)-C(35)-P(1)	117.58(19)	C(35)-C(36)-C(37)	119.9(3)
C(38)-C(37)-C(36)	120.4(3)	C(37)-C(38)-C(39)	119.9(3)
C(40)-C(39)-C(38)	120.1(3)	C(39)-C(40)-C(35)	120.3(3)
0(2)-C(41)-C(42)	108.2(5)	C(41)-C(42)-C(43)	102.3(5)
C(44)-C(43)-C(42)	101.4(5)	0(2)-C(44)-C(43)	105.9(5)
C(44A)-O(2A)-C(41A)	107.2(16)	O(1A)-C(1A)-Ru(1)	178.3(12)
C(42A)-C(41A)-O(2A)	104.0(17)	C(43A)-C(42A)-C(41A)	103.3(15)
C(44A)-C(43A)-C(42A)	108.2(14)	O(2A)-C(44A)-C(43A)	112.4(16)

Table 28. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIMes)(PPh_3)(CO)HF **(27)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	22(1)	22(1)	31(1)	0(1)	12(1)	-1(1)
P(1)	24(1)	23(1)	31(1)	0(1)	12(1)	-2(1)
F(1)	32(1)	26(1)	69(1)	-4(1)	22(1)	2(1)
O(1)	41(2)	35(1)	87(2)	-15(2)	38(2)	1(1)
0(2)	166(5)	138(5)	89(3)	35(3)	68(4)	97(4)
N(1)	27(1)	33(1)	33(1)	-3(1)	13(1)	-5(1)
N(2)	27(1)	26(1)	37(1)	-1(1)	12(1)	-4(1)
C(1)	29(2)	29(2)	42(2)	-6(2)	18(2)	-6(1)
C(2)	28(1)	25(1)	34(1)	-2(1)	15(1)	-1(1)
C(3)	31(1)	41(1)	41(1)	-7(1)	13(1)	-14(1)
C(4)	33(1)	32(1)	46(1)	-2(1)	16(1)	-10(1)
C(5)	31(1)	40(1)	32(1)	-3(1)	12(1)	-5(1)
C(6)	39(1)	52(2)	36(1)	-1(1)	14(1)	4(1)
C(7)	54(2)	65(2)	43(2)	10(1)	20(1)	15(2)
C(8)	59(2)	67(2)	39(2)	9(1)	21(1)	2(2)
C(9)	53(2)	59(2)	41(2)	-3(1)	27(1)	-2(1)
C(10)	43(1)	43(1)	40(1)	-7(1)	20(1)	-4(1)
C(11)	52(2)	75(2)	42(2)	8(1)	24(1)	27(2)
C(12)	91(3)	110(3)	55(2)	34(2)	36(2)	21(3)
C(13)	57(2)	54(2)	55(2)	-10(1)	30(2)	7(1)
C(14)	26(1)	28(1)	40(1)	6(1)	13(1)	-1(1)
C(15)	33(1)	29(1)	59(2)	13(1)	21(1)	2(1)
C(16)	28(1)	45(2)	67(2)	26(1)	17(1)	6(1)
C(17)	30(1)	62(2)	49(2)	26(1)	10(1)	-6(1)
C(18)	37(1)	54(2)	38(1)	9(1)	12(1)	-7(1)
C(19)	30(1)	35(1)	39(1)	6(1)	12(1)	-1(1)
C(20)	49(2)	32(1)	76(2)	8(1)	32(2)	10(1)
C(21)	39(2)	109(3)	53(2)	37(2)	5(1)	-4(2)
C(22)	43(1)	50(2)	42(2)	1(1)	18(1)	10(1)
C(23)	28(1)	26(1)	31(1)	1(1)	13(1)	2(1)
C(24)	35(1)	37(1)	34(1)	2(1)	14(1)	-6(1)
C(25)	52(2)	39(1)	36(1)	9(1)	15(1)	-3(1)

C(26)	42(1)	50(2)	38(1)	10(1)	15(1)	17(1)
C(27)	29(1)	70(2)	50(2)	18(1)	17(1)	10(1)
C(28)	28(1)	46(1)	45(1)	14(1)	16(1)	3(1)
C(29)	26(1)	25(1)	30(1)	1(1)	14(1)	-2(1)
C(30)	30(1)	31(1)	40(1)	-2(1)	13(1)	-4(1)
C(31)	40(1)	35(1)	47(2)	-11(1)	19(1)	-10(1)
C(32)	49(2)	24(1)	60(2)	-3(1)	33(1)	-2(1)
C(33)	40(1)	29(1)	51(2)	9(1)	22(1)	6(1)
C(34)	33(1)	27(1)	35(1)	4(1)	14(1)	0(1)
C(35)	25(1)	38(1)	29(1)	1(1)	12(1)	-4(1)
C(36)	32(1)	42(1)	36(1)	4(1)	14(1)	-5(1)
C(37)	38(1)	61(2)	43(2)	10(1)	18(1)	-10(1)
C(38)	50(2)	82(2)	41(2)	-5(2)	29(1)	-12(2)
C(39)	76(2)	66(2)	60(2)	-15(2)	46(2)	-6(2)
C(40)	61(2)	42(2)	57(2)	-7(1)	37(2)	-6(1)
C(41)	88(4)	111(6)	56(3)	0(4)	21(3)	30(4)
C(42)	61(3)	76(4)	77(4)	15(3)	18(3)	18(3)
C(43)	68(4)	101(5)	78(4)	26(4)	34(3)	35(3)
C(44)	82(4)	86(4)	70(4)	18(3)	20(3)	20(3)

Table 29. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIMes)(PPh_3)(CO)HF **(27)**.

Atom	x	y	z	U(eq)
H(3)	1063	-2402	6962	44
H(4)	1899	-2968	8056	43
H(7)	652	843	5714	63
H(9)	2740	-767	5184	58
H(11A)	290	633	6692	81
H(11B)	1258	333	7258	81
H(11C)	415	-472	6955	81
H(12A)	1877	434	4472	123
H(12B)	1594	1385	4820	123
H(12C)	736	605	4498	123
H(13A)	3696	-2009	5844	79
H(13B)	3083	-2563	6271	79
H(13C)	3930	-1770	6590	79
H(16)	5751	-3156	9408	55
H(18)	4183	-1144	10106	51
H(20A)	4083	-3103	7803	74
H(20B)	4623	-3954	8283	74
H(20C)	5286	-3094	8097	74
H(21A)	5631	-1795	10804	103
H(21B)	6511	-2056	10476	103
H(21C)	5849	-2917	10664	103
H(22A)	2269	-777	8631	65
H(22B)	2933	-76	9176	65
H(22C)	2273	-941	9360	65
H(24)	5814	-691	8892	41
H(25)	7076	-1439	9690	50
H(26)	8762	-1013	9842	51
H(27)	9195	197	9207	58
H(28)	7944	932	8387	46
H(30)	6837	2056	8939	39

H(31)	6683	3714	9167	47
H(32)	5394	4655	8528	49
H(33)	4206	3935	7669	45
H(34)	4361	2274	7429	37
H(36)	6577	2382	7334	43
H(37)	7459	2494	6553	55
H(38)	7840	1088	6064	65
H(39)	7365	-452	6360	74
H(40)	6417	-569	7098	59
H(41A)	3554	1560	6005	101
H(41B)	4614	2124	6264	101
H(42A)	4170	539	5396	86
H(42B)	5228	781	5915	86
H(43A)	5652	1964	5279	96
H(43B)	5045	1210	4736	96
H(44A)	4414	2982	4733	95
H(44B)	3607	2102	4532	95
H(1)	3890(40)	250(30)	7013(11)	112(16)
H(41C)	3401	1362	5788	129
H(41D)	4536	931	5982	129
H(42C)	3911	2853	5591	87
H(42D)	4988	2505	6048	87
H(43C)	4708	2938	4849	90
H(43D)	5618	2255	5242	90
H(44C)	4023	1767	4310	111
H(44D)	5001	1124	4639	111

Table 30. Crystal data and structure refinement for $Ru(IMes)(PPh_3)(CO)_2HF$ **(31)**.

Compound	$Ru(IMes)(PPh_3)(CO)_2HF$ **(31)**
Empirical formula	C47 H46 F N2 O2 P Ru
Formula weight	821.90
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 44.3340(5)Å α = 90°
	b = 13.7120(2)Å β = 93.960(1)°
	c = 13.3720(2)Å γ = 90°
Volume	8109.53(19) $Å^3$
Z	8
Density (calculated)	1.346 Mg/m^3
Absorption coefficient	0.471 mm^{-1}
F(000)	3408
Crystal size	0.13 x 0.10 x 0.08 mm
Theta range for data collection	3.55 to 27.48°
Index ranges	-57<=h<=53; -17<=k<=17; -17<=l<=17
Reflections collected	68050
Independent reflections	9272 [R(int) = 0.0870]
Reflections observed (>2σ)	6981
Data Completeness	0.997
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9272 / 1 / 497
Goodness-of-fit on F^2	1.043
Final R indices [I>2σ(I)]	R1 = 0.0391 wR2 = 0.0797
R indices (all data)	R1 = 0.0658 wR2 = 0.0906
Largest diff. peak and hole	0.685 and -0.596 $eÅ^{-3}$

Table 31. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IMes)(PPh_3)(CO)_2HF$ **(31)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	1370(1)	2312(1)	4474(1)	21(1)
P(1)	1503(1)	3233(1)	3089(1)	21(1)
F(1)	1326(1)	1181(1)	3450(1)	33(1)
O(1)	711(1)	3068(2)	4155(2)	54(1)
O(2)	1513(1)	3856(2)	6006(2)	41(1)
N(1)	1583(1)	678(2)	5980(2)	23(1)
N(2)	1120(1)	1023(2)	6190(2)	24(1)
C(1)	939(1)	2686(2)	4267(2)	31(1)
C(2)	1451(1)	3276(2)	5403(2)	26(1)
C(3)	1352(1)	1272(2)	5618(2)	22(1)
C(4)	1493(1)	77(2)	6744(2)	28(1)
C(5)	1205(1)	297(2)	6877(2)	29(1)
C(6)	814(1)	1370(2)	6044(2)	28(1)
C(7)	624(1)	917(2)	5301(2)	31(1)
C(8)	327(1)	1254(2)	5179(2)	37(1)
C(9)	220(1)	1990(3)	5765(2)	43(1)
C(10)	415(1)	2407(2)	6504(2)	42(1)

C(11)	715(1)	2101(2)	6661(2)	33(1)
C(12)	742(1)	144(2)	4643(2)	40(1)
C(13)	-103(1)	2341(3)	5607(3)	65(1)
C(14)	924(1)	2565(3)	7465(2)	45(1)
C(15)	1880(1)	610(2)	5599(2)	25(1)
C(16)	2112(1)	1189(2)	6024(2)	28(1)
C(17)	2395(1)	1116(2)	5634(2)	34(1)
C(18)	2446(1)	485(2)	4856(2)	39(1)
C(19)	2212(1)	-95(2)	4479(2)	36(1)
C(20)	1923(1)	-53(2)	4839(2)	31(1)
C(21)	2060(1)	1892(2)	6855(2)	36(1)
C(22)	2754(1)	443(3)	4431(3)	54(1)
C(23)	1668(1)	-691(2)	4424(2)	40(1)
C(24)	1210(1)	3392(2)	2057(2)	23(1)
C(25)	1069(1)	2556(2)	1661(2)	36(1)
C(26)	856(1)	2628(2)	850(2)	42(1)
C(27)	781(1)	3528(2)	438(2)	38(1)
C(28)	916(1)	4358(2)	837(2)	34(1)
C(29)	1130(1)	4294(2)	1645(2)	29(1)
C(30)	1618(1)	4491(2)	3351(2)	23(1)
C(31)	1421(1)	5081(2)	3854(2)	29(1)
C(32)	1484(1)	6055(2)	4021(2)	34(1)
C(33)	1746(1)	6455(2)	3688(2)	36(1)
C(34)	1945(1)	5881(2)	3211(2)	33(1)
C(35)	1884(1)	4899(2)	3043(2)	28(1)
C(36)	1810(1)	2712(2)	2405(2)	23(1)
C(37)	1871(1)	3074(2)	1468(2)	34(1)
C(38)	2104(1)	2685(2)	953(2)	40(1)
C(39)	2269(1)	1909(2)	1342(2)	33(1)
C(40)	2209(1)	1530(2)	2261(2)	31(1)
C(41)	1982(1)	1931(2)	2801(2)	27(1)
C(42)	296(1)	1061(4)	2293(3)	68(1)
C(43)	150(1)	200(3)	2392(3)	65(1)
C(44)	148(1)	1907(3)	2400(3)	73(1)
C(45)	138(1)	4799(4)	1633(4)	91(2)
C(46)	309(1)	4809(4)	2523(4)	79(1)
C(47)	-172(1)	4805(3)	1606(4)	77(1)

Table 32. Bond lengths [Å] and angles [°] for Ru(IMes)(PPh_3)$(CO)_2$HF **(31)**.

Ru(1)-H(1)	1.598(9)	C(17)-C(18)	1.384(4)
Ru(1)-C(2)	1.832(3)	C(18)-C(19)	1.374(4)
Ru(1)-C(1)	1.978(3)	C(18)-C(22)	1.516(4)
Ru(1)-F(1)	2.0697(14)	C(19)-C(20)	1.399(4)
Ru(1)-C(3)	2.097(2)	C(20)-C(23)	1.507(4)
Ru(1)-P(1)	2.3502(6)	C(24)-C(29)	1.390(4)
P(1)-C(30)	1.826(2)	C(24)-C(25)	1.392(4)
P(1)-C(36)	1.836(2)	C(25)-C(26)	1.393(4)
P(1)-C(24)	1.840(2)	C(26)-C(27)	1.382(4)
O(1)-C(1)	1.140(3)	C(27)-C(28)	1.376(4)
O(2)-C(2)	1.152(3)	C(28)-C(29)	1.391(4)
N(1)-C(3)	1.368(3)	C(30)-C(35)	1.394(3)
N(1)-C(4)	1.391(3)	C(30)-C(31)	1.396(4)
N(1)-C(15)	1.447(3)	C(31)-C(32)	1.380(4)
N(2)-C(3)	1.366(3)	C(32)-C(33)	1.384(4)

N(2)-C(5)	1.389(3)	C(33)-C(34)	1.371(4)
N(2)-C(6)	1.440(3)	C(34)-C(35)	1.388(4)
C(4)-C(5)	1.338(4)	C(36)-C(37)	1.392(4)
C(6)-C(11)	1.388(4)	C(36)-C(41)	1.398(4)
C(6)-C(7)	1.402(4)	C(37)-C(38)	1.384(4)
C(7)-C(8)	1.394(4)	C(38)-C(39)	1.375(4)
C(7)-C(12)	1.494(4)	C(39)-C(40)	1.377(4)
C(8)-C(9)	1.382(5)	C(40)-C(41)	1.391(4)
C(9)-C(10)	1.390(4)	C(42)-C(44)	1.345(6)
C(9)-C(13)	1.513(4)	C(42)-C(43)	1.357(6)
C(10)-C(11)	1.397(4)	C(43)-C(43)#1	1.383(8)
C(11)-C(14)	1.509(4)	C(44)-C(44)#1	1.360(9)
C(15)-C(20)	1.388(4)	C(45)-C(46)	1.366(7)
C(15)-C(16)	1.389(4)	C(45)-C(47)	1.372(6)
C(16)-C(17)	1.396(4)	C(46)-C(47)#1	1.349(6)
C(16)-C(21)	1.501(4)	C(47)-C(46)#1	1.349(6)
H(1)-Ru(1)-C(2)	79.7(9)	C(6)-C(11)-C(14)	121.7(2)
H(1)-Ru(1)-C(1)	170.5(9)	C(10)-C(11)-C(14)	120.7(3)
C(2)-Ru(1)-C(1)	92.88(11)	C(20)-C(15)-C(16)	122.5(2)
H(1)-Ru(1)-F(1)	94.3(9)	C(20)-C(15)-N(1)	118.5(2)
C(2)-Ru(1)-F(1)	173.94(9)	C(16)-C(15)-N(1)	119.0(2)
C(1)-Ru(1)-F(1)	93.17(9)	C(15)-C(16)-C(17)	117.8(2)
H(1)-Ru(1)-C(3)	85.0(9)	C(15)-C(16)-C(21)	121.6(2)
C(2)-Ru(1)-C(3)	90.65(10)	C(17)-C(16)-C(21)	120.6(2)
C(1)-Ru(1)-C(3)	101.20(10)	C(18)-C(17)-C(16)	121.6(3)
F(1)-Ru(1)-C(3)	88.07(8)	C(19)-C(18)-C(17)	118.6(3)
H(1)-Ru(1)-P(1)	82.4(9)	C(19)-C(18)-C(22)	121.1(3)
C(2)-Ru(1)-P(1)	95.70(8)	C(17)-C(18)-C(22)	120.3(3)
C(1)-Ru(1)-P(1)	92.44(8)	C(18)-C(19)-C(20)	122.3(3)
F(1)-Ru(1)-P(1)	84.15(4)	C(15)-C(20)-C(19)	117.1(3)
C(3)-Ru(1)-P(1)	164.65(7)	C(15)-C(20)-C(23)	120.7(2)
C(30)-P(1)-C(36)	104.89(11)	C(19)-C(20)-C(23)	122.2(3)
C(30)-P(1)-C(24)	101.83(11)	C(29)-C(24)-C(25)	119.1(2)
C(36)-P(1)-C(24)	100.37(11)	C(29)-C(24)-P(1)	123.40(19)
C(30)-P(1)-Ru(1)	115.97(8)	C(25)-C(24)-P(1)	117.5(2)
C(36)-P(1)-Ru(1)	114.73(8)	C(26)-C(25)-C(24)	120.1(3)
C(24)-P(1)-Ru(1)	116.94(8)	C(27)-C(26)-C(25)	120.3(3)
C(3)-N(1)-C(4)	111.7(2)	C(28)-C(27)-C(26)	119.9(3)
C(3)-N(1)-C(15)	126.1(2)	C(27)-C(28)-C(29)	120.2(3)
C(4)-N(1)-C(15)	122.1(2)	C(24)-C(29)-C(28)	120.4(3)
C(3)-N(2)-C(5)	111.7(2)	C(35)-C(30)-C(31)	118.7(2)
C(3)-N(2)-C(6)	125.5(2)	C(35)-C(30)-P(1)	123.58(19)
C(5)-N(2)-C(6)	122.4(2)	C(31)-C(30)-P(1)	117.68(19)
O(1)-C(1)-Ru(1)	167.6(3)	C(32)-C(31)-C(30)	120.8(2)
O(2)-C(2)-Ru(1)	176.7(2)	C(31)-C(32)-C(33)	119.8(3)
N(2)-C(3)-N(1)	103.0(2)	C(34)-C(33)-C(32)	120.1(3)
N(2)-C(3)-Ru(1)	130.20(17)	C(33)-C(34)-C(35)	120.6(3)
N(1)-C(3)-Ru(1)	126.77(17)	C(34)-C(35)-C(30)	120.0(2)
C(5)-C(4)-N(1)	106.7(2)	C(37)-C(36)-C(41)	118.6(2)
C(4)-C(5)-N(2)	106.9(2)	C(37)-C(36)-P(1)	120.5(2)
C(11)-C(6)-C(7)	122.9(2)	C(41)-C(36)-P(1)	120.88(19)
C(11)-C(6)-N(2)	119.4(2)	C(38)-C(37)-C(36)	120.6(3)
C(7)-C(6)-N(2)	117.6(2)	C(39)-C(38)-C(37)	120.4(3)
C(8)-C(7)-C(6)	116.9(3)	C(38)-C(39)-C(40)	119.8(3)

C(8)-C(7)-C(12)	122.1(3)	C(39)-C(40)-C(41)	120.4(3)
C(6)-C(7)-C(12)	121.0(2)	C(40)-C(41)-C(36)	120.1(2)
C(9)-C(8)-C(7)	122.2(3)	C(44)-C(42)-C(43)	120.1(4)
C(8)-C(9)-C(10)	118.9(3)	C(42)-C(43)-C(43)#1	119.5(3)
C(8)-C(9)-C(13)	120.7(3)	C(42)-C(44)-C(44)#1	120.4(3)
C(10)-C(9)-C(13)	120.3(3)	C(46)-C(45)-C(47)	121.1(4)
C(9)-C(10)-C(11)	121.5(3)	C(47)#1-C(46)-C(45)	119.9(4)
C(6)-C(11)-C(10)	117.6(3)	C(46)#1-C(47)-C(45)	119.0(5)

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2

Table 33. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IMes)(PPh_3)(CO)_2HF$ **(31)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	23(1)	18(1)	20(1)	1(1)	2(1)	0(1)
P(1)	22(1)	20(1)	21(1)	1(1)	1(1)	0(1)
F(1)	49(1)	25(1)	26(1)	-5(1)	1(1)	-1(1)
O(1)	30(1)	64(2)	70(2)	26(1)	6(1)	12(1)
O(2)	57(1)	32(1)	34(1)	-10(1)	-2(1)	3(1)
N(1)	30(1)	18(1)	21(1)	3(1)	1(1)	1(1)
N(2)	25(1)	25(1)	24(1)	5(1)	1(1)	0(1)
C(1)	28(1)	32(2)	31(1)	8(1)	3(1)	-5(1)
C(2)	29(1)	26(2)	24(1)	3(1)	2(1)	4(1)
C(3)	28(1)	18(1)	18(1)	-1(1)	-2(1)	0(1)
C(4)	34(2)	25(1)	24(1)	6(1)	-1(1)	1(1)
C(5)	33(1)	29(2)	25(1)	10(1)	1(1)	-4(1)
C(6)	25(1)	33(2)	27(1)	7(1)	3(1)	-2(1)
C(7)	30(1)	33(2)	29(1)	8(1)	2(1)	-6(1)
C(8)	27(2)	50(2)	34(2)	8(1)	-2(1)	-9(1)
C(9)	27(2)	61(2)	41(2)	12(2)	4(1)	4(1)
C(10)	33(2)	55(2)	37(2)	0(1)	9(1)	7(1)
C(11)	29(1)	44(2)	26(1)	3(1)	4(1)	1(1)
C(12)	40(2)	37(2)	40(2)	-3(1)	-5(1)	-6(1)
C(13)	30(2)	97(3)	67(2)	1(2)	-2(2)	15(2)
C(14)	42(2)	58(2)	36(2)	-13(2)	2(1)	3(1)
C(15)	28(1)	23(1)	24(1)	6(1)	3(1)	6(1)
C(16)	28(1)	29(2)	27(1)	6(1)	2(1)	5(1)
C(17)	25(1)	43(2)	36(2)	12(1)	2(1)	5(1)
C(18)	35(2)	47(2)	34(2)	16(1)	9(1)	17(1)
C(19)	49(2)	34(2)	28(1)	5(1)	8(1)	17(1)
C(20)	40(2)	25(2)	27(1)	4(1)	0(1)	9(1)
C(21)	33(2)	37(2)	38(2)	-5(1)	-1(1)	-1(1)
C(22)	38(2)	79(3)	47(2)	18(2)	14(1)	21(2)
C(23)	51(2)	30(2)	39(2)	-7(1)	0(1)	7(1)
C(24)	21(1)	28(1)	21(1)	2(1)	2(1)	0(1)
C(25)	39(2)	30(2)	37(2)	3(1)	-6(1)	-3(1)
C(26)	41(2)	41(2)	42(2)	-6(1)	-12(1)	-8(1)
C(27)	29(2)	51(2)	32(2)	6(1)	-7(1)	-1(1)
C(28)	32(2)	36(2)	34(2)	13(1)	-1(1)	4(1)
C(29)	30(1)	27(2)	30(1)	6(1)	1(1)	-4(1)
C(30)	28(1)	20(1)	18(1)	3(1)	-2(1)	-1(1)
C(31)	34(2)	25(2)	30(1)	0(1)	6(1)	1(1)

C(32)	46(2)	27(2)	29(1)	-2(1)	4(1)	4(1)
C(33)	56(2)	21(2)	29(1)	3(1)	-4(1)	-8(1)
C(34)	36(2)	31(2)	32(2)	5(1)	-1(1)	-10(1)
C(35)	28(1)	30(2)	26(1)	1(1)	1(1)	-3(1)
C(36)	23(1)	24(1)	24(1)	-1(1)	1(1)	-1(1)
C(37)	34(2)	41(2)	27(1)	2(1)	2(1)	10(1)
C(38)	40(2)	58(2)	22(1)	3(1)	6(1)	8(1)
C(39)	26(1)	44(2)	31(2)	-9(1)	3(1)	5(1)
C(40)	26(1)	28(2)	40(2)	-4(1)	1(1)	5(1)
C(41)	25(1)	26(1)	29(1)	1(1)	3(1)	0(1)
C(42)	55(2)	97(4)	53(2)	13(2)	5(2)	3(2)
C(43)	106(3)	53(2)	34(2)	-5(2)	-7(2)	31(2)
C(44)	101(3)	58(3)	56(2)	15(2)	-21(2)	-27(2)
C(45)	77(3)	115(4)	83(3)	15(3)	31(3)	19(3)
C(46)	56(3)	86(3)	97(4)	-1(3)	22(2)	5(2)
C(47)	73(3)	77(3)	81(3)	14(2)	9(2)	4(2)

Table 34. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(IMes)(PPh_3)$(CO)_2$HF **(31)**.

Atom	x	y	z	U(eq)
H(4)	1614	-398	7102	34
H(5)	1082	11	7351	35
H(8)	193	967	4676	45
H(10)	343	2912	6911	50
H(12A)	884	434	4199	59
H(12B)	573	-152	4240	59
H(12C)	846	-358	5060	59
H(13A)	-151	2467	4893	97
H(13B)	-128	2942	5989	97
H(13C)	-240	1839	5838	97
H(14A)	979	2081	7985	68
H(14B)	821	3114	7762	68
H(14C)	1107	2799	7169	68
H(17)	2556	1509	5910	41
H(19)	2248	-540	3956	44
H(21A)	1938	2442	6589	54
H(21B)	2255	2133	7144	54
H(21C)	1953	1561	7375	54
H(22A)	2897	110	4907	81
H(22B)	2825	1107	4316	81
H(22C)	2738	86	3795	81
H(23A)	1598	-1102	4961	60
H(23B)	1738	-1105	3891	60
H(23C)	1501	-280	4152	60
H(25)	1119	1936	1945	43
H(26)	761	2055	579	50
H(27)	637	3573	-120	45
H(28)	862	4978	561	41
H(29)	1223	4870	1916	35
H(31)	1241	4809	4083	35
H(32)	1349	6450	4365	41
H(33)	1788	7129	3790	43
H(34)	2125	6158	2993	40

H(35)	2024	4505	2718	33
H(37)	1753	3593	1179	40
H(38)	2149	2956	327	47
H(39)	2425	1636	979	40
H(40)	2322	992	2528	38
H(41)	1944	1674	3440	32
H(42)	503	1066	2148	82
H(43)	254	-399	2313	78
H(44)	252	2509	2335	88
H(45)	235	4788	1022	109
H(46)	523	4819	2529	95
H(47)	-289	4806	983	92
H(1)	1728(2)	2201(19)	4653(19)	23(7)

Table 35. Crystal data and structure refinement for Ru(SIMes)(PPh_3)(CO)HF **(32)**.

Compound	Ru(SIMes)(PPh_3)(CO)HF **(32)**
Empirical formula	C40 H42 F N2 O P Ru
Formula weight	717.80
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/a$
Unit cell dimensions	a = 15.1040(2)Å α = 90°
	b = 14.1360(2)Å β = 99.633(1)°
	c = 16.7450(3)Å γ = 90°
Volume	3524.82(9) $Å^3$
Z	4
Density (calculated)	1.353 Mg/m^3
Absorption coefficient	0.529 mm^{-1}
F(000)	1488
Crystal size	0.25 x 0.20 x 0.12 mm
Theta range for data collection	3.70 to 27.47°
Index ranges	-18<=h<=19; -18<=k<=18; -21<=l<=21
Reflections collected	56161
Independent reflections	8060 [R(int) = 0.0564]
Reflections observed (>2σ)	6642
Data Completeness	0.996
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.94 and 0.89
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8060 / 2 / 430
Goodness-of-fit on F^2	1.071
Final R indices [I>2σ(I)]	R1 = 0.0318 wR2 = 0.0729
R indices (all data)	R1 = 0.0443 wR2 = 0.0787
Largest diff. peak and hole	0.677 and -0.547 $eÅ^{-3}$

Table 36. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIMes)(PPh_3)(CO)HF **(32)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	2173(1)	5676(1)	7553(1)	24(1)
P(1)	1096(1)	4462(1)	7362(1)	25(1)
F(1)	2849(1)	4765(1)	8361(1)	45(1)
O(1)	1143(1)	7140(1)	6519(1)	47(1)
N(1)	4034(1)	6342(1)	7439(1)	29(1)
C(1)	1544(2)	6550(2)	6913(1)	32(1)
N(2)	3486(1)	7263(1)	8270(1)	28(1)
C(2)	3305(1)	6525(1)	7767(1)	27(1)
C(3)	4767(2)	7029(2)	7680(2)	35(1)
C(4)	4430(1)	7586(2)	8350(1)	32(1)
C(5)	4051(1)	5699(2)	6780(1)	31(1)
C(6)	4380(2)	4780(2)	6939(2)	35(1)
C(7)	4396(2)	4179(2)	6281(2)	41(1)
C(8)	4088(2)	4459(2)	5490(2)	43(1)
C(9)	3777(2)	5373(2)	5355(2)	43(1)
C(10)	3758(2)	6010(2)	5988(2)	37(1)
C(11)	4673(2)	4438(2)	7789(2)	43(1)
C(12)	4074(2)	3777(2)	4793(2)	58(1)
C(13)	3437(2)	7009(2)	5809(2)	48(1)
C(14)	2865(1)	7698(1)	8721(1)	28(1)
C(15)	2421(2)	8518(2)	8408(1)	31(1)
C(16)	1825(2)	8936(2)	8851(1)	35(1)
C(17)	1654(1)	8561(2)	9576(1)	34(1)
C(18)	2129(2)	7759(2)	9874(1)	36(1)
C(19)	2742(2)	7314(2)	9463(1)	32(1)
C(20)	2568(2)	8936(2)	7612(2)	44(1)
C(21)	976(2)	9002(2)	10031(2)	45(1)
C(22)	3252(2)	6454(2)	9814(2)	46(1)
C(23)	1639(1)	3343(1)	7176(1)	30(1)
C(24)	2265(2)	3335(2)	6656(2)	38(1)
C(25)	2665(2)	2498(2)	6475(2)	42(1)
C(26)	2457(2)	1660(2)	6817(2)	46(1)
C(27)	1856(2)	1662(2)	7349(2)	61(1)
C(28)	1448(2)	2498(2)	7531(2)	48(1)
C(29)	536(1)	4183(2)	8223(1)	29(1)
C(30)	1026(2)	4264(2)	8998(1)	35(1)
C(31)	632(2)	4035(2)	9665(2)	44(1)
C(32)	-249(2)	3737(2)	9564(2)	50(1)
C(33)	-738(2)	3655(2)	8795(2)	59(1)
C(34)	-345(2)	3877(2)	8126(2)	47(1)
C(35)	156(1)	4534(1)	6519(1)	26(1)
C(36)	-8(2)	3863(2)	5911(1)	35(1)
C(37)	-727(2)	3955(2)	5281(2)	42(1)
C(38)	-1303(2)	4714(2)	5263(1)	39(1)
C(39)	-1155(2)	5388(2)	5867(2)	39(1)
C(40)	-420(2)	5306(2)	6485(1)	32(1)

Table 37. Bond lengths [Å] and angles [°] for Ru(SIMes)(PPh_3)(CO)HF **(32)**.

Ru(1)-H(1A)	1.584(19)	Ru(1)-H(1)	1.588(19)
Ru(1)-C(1)	1.800(2)	Ru(1)-F(1)	2.0172(13)
Ru(1)-C(2)	2.071(2)	Ru(1)-P(1)	2.3494(5)
P(1)-C(35)	1.830(2)	P(1)-C(23)	1.832(2)
P(1)-C(29)	1.832(2)	O(1)-C(1)	1.167(3)
N(1)-C(2)	1.334(3)	N(1)-C(5)	1.433(3)
N(1)-C(3)	1.477(3)	N(2)-C(2)	1.340(3)
N(2)-C(14)	1.437(3)	N(2)-C(4)	1.481(3)
C(3)-C(4)	1.525(3)	C(5)-C(10)	1.398(3)
C(5)-C(6)	1.400(3)	C(6)-C(7)	1.394(3)
C(6)-C(11)	1.499(4)	C(7)-C(8)	1.387(4)
C(8)-C(9)	1.381(4)	C(8)-C(12)	1.511(3)
C(9)-C(10)	1.394(3)	C(10)-C(13)	1.507(3)
C(14)-C(19)	1.396(3)	C(14)-C(15)	1.396(3)
C(15)-C(16)	1.391(3)	C(15)-C(20)	1.509(3)
C(16)-C(17)	1.387(3)	C(17)-C(18)	1.389(3)
C(17)-C(21)	1.510(3)	C(18)-C(19)	1.393(3)
C(19)-C(22)	1.505(3)	C(23)-C(28)	1.386(3)
C(23)-C(24)	1.389(3)	C(24)-C(25)	1.385(3)
C(25)-C(26)	1.374(4)	C(26)-C(27)	1.374(4)
C(27)-C(28)	1.390(4)	C(29)-C(34)	1.383(3)
C(29)-C(30)	1.388(3)	C(30)-C(31)	1.388(3)
C(31)-C(32)	1.380(4)	C(32)-C(33)	1.377(4)
C(33)-C(34)	1.389(4)	C(35)-C(36)	1.382(3)
C(35)-C(40)	1.391(3)	C(36)-C(37)	1.388(3)
C(37)-C(38)	1.377(4)	C(38)-C(39)	1.381(3)
C(39)-C(40)	1.390(3)		
H(1A)-Ru(1)-H(1)	151(2)	H(1A)-Ru(1)-C(1)	77.5(18)
H(1)-Ru(1)-C(1)	75.9(16)	H(1A)-Ru(1)-F(1)	97.4(18)
H(1)-Ru(1)-F(1)	109.4(16)	C(1)-Ru(1)-F(1)	174.64(8)
H(1A)-Ru(1)-C(2)	98.5(19)	H(1)-Ru(1)-C(2)	93.0(16)
C(1)-Ru(1)-C(2)	92.51(9)	F(1)-Ru(1)-C(2)	86.75(7)
H(1A)-Ru(1)-P(1)	88.8(19)	H(1)-Ru(1)-P(1)	84.5(16)
C(1)-Ru(1)-P(1)	97.81(7)	F(1)-Ru(1)-P(1)	83.45(4)
C(2)-Ru(1)-P(1)	168.44(6)	C(35)-P(1)-C(23)	103.20(10)
C(35)-P(1)-C(29)	102.61(10)	C(23)-P(1)-C(29)	103.08(10)
C(35)-P(1)-Ru(1)	119.64(7)	C(23)-P(1)-Ru(1)	109.56(7)
C(29)-P(1)-Ru(1)	116.76(7)	C(2)-N(1)-C(5)	124.14(18)
C(2)-N(1)-C(3)	113.15(17)	C(5)-N(1)-C(3)	121.19(17)
O(1)-C(1)-Ru(1)	177.6(2)	C(2)-N(2)-C(14)	125.53(17)
C(2)-N(2)-C(4)	112.87(17)	C(14)-N(2)-C(4)	121.56(17)
N(1)-C(2)-N(2)	108.25(18)	N(1)-C(2)-Ru(1)	122.11(15)
N(2)-C(2)-Ru(1)	129.44(15)	N(1)-C(3)-C(4)	102.26(17)
N(2)-C(4)-C(3)	102.09(16)	C(10)-C(5)-C(6)	121.2(2)
C(10)-C(5)-N(1)	119.18(19)	C(6)-C(5)-N(1)	119.6(2)
C(7)-C(6)-C(5)	117.9(2)	C(7)-C(6)-C(11)	120.8(2)
C(5)-C(6)-C(11)	121.2(2)	C(8)-C(7)-C(6)	122.3(2)
C(9)-C(8)-C(7)	118.2(2)	C(9)-C(8)-C(12)	120.8(3)
C(7)-C(8)-C(12)	121.0(2)	C(8)-C(9)-C(10)	122.0(2)
C(9)-C(10)-C(5)	118.3(2)	C(9)-C(10)-C(13)	120.0(2)
C(5)-C(10)-C(13)	121.6(2)	C(19)-C(14)-C(15)	121.9(2)
C(19)-C(14)-N(2)	119.87(19)	C(15)-C(14)-N(2)	118.16(19)

C(16)-C(15)-C(14)	117.8(2)	C(16)-C(15)-C(20)	120.6(2)
C(14)-C(15)-C(20)	121.7(2)	C(17)-C(16)-C(15)	122.4(2)
C(16)-C(17)-C(18)	117.8(2)	C(16)-C(17)-C(21)	121.7(2)
C(18)-C(17)-C(21)	120.6(2)	C(17)-C(18)-C(19)	122.4(2)
C(18)-C(19)-C(14)	117.6(2)	C(18)-C(19)-C(22)	120.7(2)
C(14)-C(19)-C(22)	121.7(2)	C(28)-C(23)-C(24)	118.3(2)
C(28)-C(23)-P(1)	122.72(17)	C(24)-C(23)-P(1)	118.98(16)
C(25)-C(24)-C(23)	120.8(2)	C(26)-C(25)-C(24)	120.4(2)
C(25)-C(26)-C(27)	119.4(2)	C(26)-C(27)-C(28)	120.6(2)
C(23)-C(28)-C(27)	120.5(2)	C(34)-C(29)-C(30)	119.1(2)
C(34)-C(29)-P(1)	122.53(18)	C(30)-C(29)-P(1)	118.30(17)
C(29)-C(30)-C(31)	120.0(2)	C(32)-C(31)-C(30)	120.5(2)
C(33)-C(32)-C(31)	119.7(2)	C(32)-C(33)-C(34)	120.0(3)
C(29)-C(34)-C(33)	120.7(2)	C(36)-C(35)-C(40)	118.3(2)
C(36)-C(35)-P(1)	123.37(17)	C(40)-C(35)-P(1)	118.32(16)
C(35)-C(36)-C(37)	121.1(2)	C(38)-C(37)-C(36)	120.0(2)
C(37)-C(38)-C(39)	119.8(2)	C(38)-C(39)-C(40)	119.9(2)
C(39)-C(40)-C(35)	120.9(2)		

Table 38. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIMes)(PPh_3)(CO)HF **(32)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	23(1)	21(1)	27(1)	-1(1)	3(1)	0(1)
P(1)	24(1)	22(1)	29(1)	1(1)	4(1)	-1(1)
F(1)	34(1)	42(1)	55(1)	17(1)	-7(1)	-2(1)
O(1)	48(1)	38(1)	52(1)	16(1)	-5(1)	2(1)
N(1)	24(1)	26(1)	38(1)	-6(1)	4(1)	-3(1)
C(1)	31(1)	30(1)	34(1)	0(1)	2(1)	-6(1)
N(2)	26(1)	25(1)	34(1)	-4(1)	3(1)	-3(1)
C(2)	26(1)	23(1)	31(1)	3(1)	0(1)	2(1)
C(3)	28(1)	34(1)	44(1)	-8(1)	4(1)	-5(1)
C(4)	27(1)	31(1)	38(1)	-5(1)	3(1)	-6(1)
C(5)	28(1)	26(1)	37(1)	-7(1)	3(1)	-2(1)
C(6)	28(1)	29(1)	48(1)	-3(1)	7(1)	1(1)
C(7)	34(1)	30(1)	59(2)	-11(1)	12(1)	-1(1)
C(8)	38(1)	41(1)	52(2)	-18(1)	13(1)	-9(1)
C(9)	42(1)	47(1)	39(1)	-8(1)	4(1)	-6(1)
C(10)	36(1)	34(1)	40(1)	-5(1)	4(1)	0(1)
C(11)	40(1)	34(1)	56(2)	2(1)	10(1)	6(1)
C(12)	61(2)	55(2)	61(2)	-30(1)	17(2)	-13(1)
C(13)	60(2)	42(1)	40(1)	3(1)	4(1)	8(1)
C(14)	27(1)	25(1)	31(1)	-4(1)	4(1)	-2(1)
C(15)	34(1)	26(1)	31(1)	-3(1)	2(1)	-3(1)
C(16)	34(1)	27(1)	40(1)	-5(1)	-2(1)	4(1)
C(17)	25(1)	36(1)	41(1)	-13(1)	3(1)	-4(1)
C(18)	36(1)	40(1)	32(1)	-2(1)	9(1)	-6(1)
C(19)	31(1)	30(1)	34(1)	0(1)	2(1)	-2(1)
C(20)	58(2)	35(1)	39(1)	8(1)	6(1)	7(1)
C(21)	34(1)	51(2)	52(2)	-20(1)	9(1)	-2(1)
C(22)	55(2)	40(1)	44(1)	12(1)	10(1)	9(1)
C(23)	25(1)	25(1)	39(1)	0(1)	2(1)	0(1)
C(24)	39(1)	28(1)	50(1)	-2(1)	14(1)	1(1)

C(25)	37(1)	38(1)	53(2)	-9(1)	12(1)	3(1)
C(26)	37(1)	28(1)	70(2)	-8(1)	4(1)	7(1)
C(27)	64(2)	23(1)	103(3)	10(1)	32(2)	6(1)
C(28)	46(1)	29(1)	75(2)	9(1)	27(1)	4(1)
C(29)	30(1)	27(1)	32(1)	3(1)	6(1)	1(1)
C(30)	33(1)	38(1)	34(1)	4(1)	4(1)	2(1)
C(31)	49(2)	49(1)	32(1)	7(1)	5(1)	6(1)
C(32)	49(2)	63(2)	40(1)	17(1)	16(1)	4(1)
C(33)	38(1)	89(2)	51(2)	25(2)	10(1)	-10(1)
C(34)	37(1)	68(2)	36(1)	14(1)	3(1)	-11(1)
C(35)	25(1)	25(1)	29(1)	2(1)	5(1)	-5(1)
C(36)	36(1)	31(1)	39(1)	-7(1)	5(1)	-1(1)
C(37)	44(1)	44(1)	35(1)	-9(1)	3(1)	-11(1)
C(38)	36(1)	45(1)	33(1)	9(1)	-4(1)	-10(1)
C(39)	32(1)	35(1)	47(1)	8(1)	-1(1)	2(1)
C(40)	33(1)	27(1)	36(1)	-2(1)	4(1)	0(1)

Table 39. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIMes)(PPh_3)(CO)HF **(32)**.

Atom	x	y	z	U(eq)
H(1)	2330(30)	5400(30)	6668(15)	29(12)
H(18A)	4849	7444	7222	42
H(18B)	5341	6704	7886	42
H(21A)	4774	7427	8889	39
H(21B)	4464	8276	8259	39
H(31)	4625	3556	6379	49
H(29)	3570	5575	4815	51
H(12A)	5116	4878	8078	64
H(12B)	4942	3809	7779	64
H(12C)	4151	4404	8067	64
H(53A)	3495	3449	4691	87
H(53B)	4558	3313	4929	87
H(53C)	4161	4126	4306	87
H(37A)	3020	7185	6173	71
H(37B)	3130	7051	5246	71
H(37C)	3952	7440	5890	71
H(15)	1523	9498	8650	41
H(28)	2032	7504	10377	43
H(32A)	3101	9342	7701	66
H(32B)	2042	9311	7380	66
H(32C)	2656	8425	7237	66
H(24A)	1290	9316	10519	68
H(24B)	581	8509	10185	68
H(24C)	617	9468	9684	68
H(36A)	3891	6611	9960	69
H(36B)	3177	5944	9412	69
H(36C)	3020	6248	10298	69
H(22)	2420	3911	6421	46
H(26)	3087	2503	6113	51
H(44)	2726	1086	6686	55
H(33)	1717	1086	7594	74
H(34)	1036	2490	7902	58
H(23)	1631	4476	9073	42

H(38)	972	4085	10194	52
H(46)	-518	3589	10022	60
H(47)	-1344	3445	8723	71
H(40)	-685	3819	7598	57
H(30)	378	3330	5925	42
H(42)	-823	3494	4862	50
H(35)	-1799	4773	4835	47
H(43)	-1556	5907	5860	47
H(16)	-310	5782	6889	38
H(1A)	1610(30)	6180(30)	8150(30)	44(14)

Table 40. Crystal data and structure refinement for Ru(SIMes)(PPh_3)$(CO)_2$HF **(34)**.

Compound	Ru(SIMes)(PPh_3)$(CO)_2$HF **(34)**.
Empirical formula	C47 H48 F N2 O2 P Ru
Formula weight	823.91
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 44.3450(5)Å α = 90°
	b = 13.66400(10)Å β = 93.8370(10)°
	c = 13.47900(10)Å γ = 90°
Volume	8149.02(13) $Å^3$
Z	8
Density (calculated)	1.343 Mg/m^3
Absorption coefficient	0.469 mm^{-1}
F(000)	3424
Crystal size	0.15 x 0.13 x 0.10 mm
Theta range for data collection	3.55 to 27.48 °.
Index ranges	-57<=h<=57; -17<=k<=17; -17<=l<=17
Reflections collected	79799
Independent reflections	9313 [R(int) = 0.0574]
Reflections observed (>2σ)	7541
Data Completeness	0.997
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.97 and 0.93
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9313 / 1 / 494
Goodness-of-fit on F^2	1.023
Final R indices [I>2σ(I)]	R^1 = 0.0340 wR2 = 0.0753
R indices (all data)	R^1 = 0.0492 wR2 = 0.0822
Largest diff. peak and hole	0.593 and -0.601 $eÅ^{-3}$

Table 41. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIMes)(PPh_3)$(CO)_2$HF **(34)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	1375(1)	2287(1)	4497(1)	19(1)
P(1)	1505(1)	3222(1)	3120(1)	20(1)
F(1)	1336(1)	1153(1)	3478(1)	31(1)
O(1)	719(1)	3059(2)	4172(2)	56(1)
O(2)	1516(1)	3840(1)	6017(1)	42(1)

N(1)	1585(1)	657(1)	5960(1)	23(1)
N(2)	1124(1)	1064(1)	6209(1)	25(1)
C(1)	945(1)	2664(2)	4289(2)	31(1)
C(2)	1454(1)	3252(2)	5420(2)	27(1)
C(3)	1357(1)	1249(2)	5645(2)	20(1)
C(4)	1510(1)	-23(2)	6763(2)	27(1)
C(5)	1190(1)	292(2)	6962(2)	32(1)
C(6)	1880(1)	591(2)	5575(2)	23(1)
C(7)	1926(1)	-89(2)	4824(2)	28(1)
C(8)	2213(1)	-138(2)	4465(2)	34(1)
C(9)	2449(1)	448(2)	4833(2)	36(1)
C(10)	2397(1)	1091(2)	5602(2)	33(1)
C(11)	2116(1)	1167(2)	5993(2)	27(1)
C(12)	1671(1)	-727(2)	4416(2)	36(1)
C(13)	2757(1)	403(3)	4414(2)	52(1)
C(14)	2066(1)	1881(2)	6812(2)	35(1)
C(15)	819(1)	1399(2)	6040(2)	26(1)
C(16)	714(1)	2144(2)	6635(2)	32(1)
C(17)	413(1)	2424(2)	6471(2)	40(1)
C(18)	220(1)	1982(2)	5750(2)	41(1)
C(19)	332(1)	1239(2)	5183(2)	38(1)
C(20)	632(1)	927(2)	5313(2)	29(1)
C(21)	917(1)	2639(2)	7426(2)	43(1)
C(22)	-105(1)	2314(3)	5579(3)	63(1)
C(23)	753(1)	142(2)	4672(2)	39(1)
C(24)	1809(1)	2698(2)	2429(2)	22(1)
C(25)	1983(1)	1919(2)	2820(2)	28(1)
C(26)	2209(1)	1516(2)	2278(2)	32(1)
C(27)	2267(1)	1887(2)	1360(2)	33(1)
C(28)	2098(1)	2663(2)	973(2)	37(1)
C(29)	1868(1)	3058(2)	1494(2)	32(1)
C(30)	1620(1)	4486(2)	3373(2)	22(1)
C(31)	1885(1)	4892(2)	3061(2)	26(1)
C(32)	1946(1)	5881(2)	3216(2)	32(1)
C(33)	1747(1)	6464(2)	3691(2)	35(1)
C(34)	1487(1)	6065(2)	4026(2)	34(1)
C(35)	1424(1)	5080(2)	3871(2)	28(1)
C(36)	1210(1)	3388(2)	2110(2)	23(1)
C(37)	1143(1)	4284(2)	1659(2)	28(1)
C(38)	927(1)	4346(2)	865(2)	34(1)
C(39)	779(1)	3516(2)	511(2)	37(1)
C(40)	842(1)	2620(2)	963(2)	40(1)
C(41)	1055(1)	2555(2)	1764(2)	33(1)
C(42)	137(1)	5217(4)	6633(4)	89(1)
C(43)	310(1)	5224(3)	7517(4)	80(1)
C(44)	174(1)	5225(3)	8385(3)	79(1)
C(45)	149(1)	8119(3)	7434(3)	60(1)
C(46)	301(1)	8983(3)	7361(3)	65(1)
C(47)	142(1)	9855(3)	7424(2)	66(1)

Table 42. Bond lengths [Å] and angles [°] for Ru(SIMes)(PPh_3)$(CO)_2$HF **(34)**.

Ru(1)-C(2)	1.830(2)	C(18)-C(19)	1.383(4)
Ru(1)-C(1)	1.977(3)	C(18)-C(22)	1.514(4)
Ru(1)-F(1)	2.0704(13)	C(19)-C(20)	1.396(4)
Ru(1)-C(3)	2.106(2)	C(20)-C(23)	1.499(4)
Ru(1)-P(1)	2.3565(6)	C(24)-C(29)	1.392(3)
P(1)-C(30)	1.827(2)	C(24)-C(25)	1.396(3)
P(1)-C(24)	1.833(2)	C(25)-C(26)	1.392(3)
P(1)-C(36)	1.838(2)	C(26)-C(27)	1.378(4)
O(1)-C(1)	1.141(3)	C(27)-C(28)	1.380(4)
O(2)-C(2)	1.157(3)	C(28)-C(29)	1.388(3)
N(1)-C(3)	1.341(3)	C(30)-C(31)	1.389(3)
N(1)-C(6)	1.440(3)	C(30)-C(35)	1.395(3)
N(1)-C(4)	1.481(3)	C(31)-C(32)	1.392(3)
N(2)-C(3)	1.347(3)	C(32)-C(33)	1.376(4)
N(2)-C(15)	1.434(3)	C(33)-C(34)	1.378(4)
N(2)-C(5)	1.479(3)	C(34)-C(35)	1.387(3)
C(4)-C(5)	1.524(3)	C(36)-C(37)	1.390(3)
C(6)-C(11)	1.398(3)	C(36)-C(41)	1.395(3)
C(6)-C(7)	1.399(3)	C(37)-C(38)	1.390(3)
C(7)-C(8)	1.393(3)	C(38)-C(39)	1.380(4)
C(7)-C(12)	1.502(4)	C(39)-C(40)	1.388(4)
C(8)-C(9)	1.385(4)	C(40)-C(41)	1.389(4)
C(9)-C(10)	1.390(4)	C(42)-C(43)	1.372(6)
C(9)-C(13)	1.512(4)	C(42)-C(44)#1	1.375(6)
C(10)-C(11)	1.391(3)	C(43)-C(44)	1.353(6)
C(11)-C(14)	1.500(3)	C(44)-C(42)#1	1.375(6)
C(15)-C(16)	1.395(3)	C(45)-C(45)#1	1.343(7)
C(15)-C(20)	1.398(3)	C(45)-C(46)	1.367(5)
C(16)-C(17)	1.395(4)	C(46)-C(47)	1.391(5)
C(16)-C(21)	1.507(4)	C(47)-C(47)#1	1.290(7)
C(17)-C(18)	1.387(4)		
C(2)-Ru(1)-C(1)	92.71(11)	C(16)-C(15)-N(2)	119.3(2)
C(2)-Ru(1)-F(1)	173.66(9)	C(20)-C(15)-N(2)	118.3(2)
C(1)-Ru(1)-F(1)	93.62(9)	C(17)-C(16)-C(15)	117.5(2)
C(2)-Ru(1)-C(3)	90.04(9)	C(17)-C(16)-C(21)	120.6(2)
C(1)-Ru(1)-C(3)	101.31(9)	C(15)-C(16)-C(21)	121.9(2)
F(1)-Ru(1)-C(3)	88.67(7)	C(18)-C(17)-C(16)	122.0(3)
C(2)-Ru(1)-P(1)	95.70(7)	C(19)-C(18)-C(17)	118.8(2)
C(1)-Ru(1)-P(1)	91.87(7)	C(19)-C(18)-C(22)	120.5(3)
F(1)-Ru(1)-P(1)	84.14(4)	C(17)-C(18)-C(22)	120.7(3)
C(3)-Ru(1)-P(1)	165.37(6)	C(18)-C(19)-C(20)	121.9(2)
C(30)-P(1)-C(24)	105.00(10)	C(19)-C(20)-C(15)	117.5(2)
C(30)-P(1)-C(36)	101.43(10)	C(19)-C(20)-C(23)	121.4(2)
C(24)-P(1)-C(36)	100.51(10)	C(15)-C(20)-C(23)	121.1(2)
C(30)-P(1)-Ru(1)	116.44(7)	C(29)-C(24)-C(25)	118.7(2)
C(24)-P(1)-Ru(1)	114.56(7)	C(29)-C(24)-P(1)	120.60(18)
C(36)-P(1)-Ru(1)	116.75(7)	C(25)-C(24)-P(1)	120.72(17)
C(3)-N(1)-C(6)	127.31(18)	C(26)-C(25)-C(24)	120.1(2)
C(3)-N(1)-C(4)	114.02(18)	C(27)-C(26)-C(25)	120.6(2)
C(6)-N(1)-C(4)	118.60(17)	C(26)-C(27)-C(28)	119.6(2)
C(3)-N(2)-C(15)	127.09(18)	C(27)-C(28)-C(29)	120.4(2)
C(3)-N(2)-C(5)	113.49(18)	C(28)-C(29)-C(24)	120.6(2)

C(15)-N(2)-C(5)	118.43(18)	C(31)-C(30)-C(35)	118.8(2)
O(1)-C(1)-Ru(1)	166.8(2)	C(31)-C(30)-P(1)	123.50(17)
O(2)-C(2)-Ru(1)	176.9(2)	C(35)-C(30)-P(1)	117.66(17)
N(1)-C(3)-N(2)	107.36(18)	C(30)-C(31)-C(32)	120.0(2)
N(1)-C(3)-Ru(1)	125.09(15)	C(33)-C(32)-C(31)	120.6(2)
N(2)-C(3)-Ru(1)	127.53(16)	C(32)-C(33)-C(34)	119.9(2)
N(1)-C(4)-C(5)	102.18(17)	C(33)-C(34)-C(35)	120.0(2)
N(2)-C(5)-C(4)	102.81(18)	C(34)-C(35)-C(30)	120.6(2)
C(11)-C(6)-C(7)	121.6(2)	C(37)-C(36)-C(41)	119.1(2)
C(11)-C(6)-N(1)	119.5(2)	C(37)-C(36)-P(1)	123.62(17)
C(7)-C(6)-N(1)	118.8(2)	C(41)-C(36)-P(1)	117.28(17)
C(8)-C(7)-C(6)	117.7(2)	C(38)-C(37)-C(36)	120.5(2)
C(8)-C(7)-C(12)	121.8(2)	C(39)-C(38)-C(37)	120.3(2)
C(6)-C(7)-C(12)	120.5(2)	C(38)-C(39)-C(40)	119.6(2)
C(9)-C(8)-C(7)	122.4(2)	C(39)-C(40)-C(41)	120.4(2)
C(8)-C(9)-C(10)	118.2(2)	C(40)-C(41)-C(36)	120.1(2)
C(8)-C(9)-C(13)	121.6(3)	C(43)-C(42)-C(44)#1	121.0(4)
C(10)-C(9)-C(13)	120.3(3)	C(44)-C(43)-C(42)	119.7(4)
C(9)-C(10)-C(11)	121.9(2)	C(43)-C(44)-C(42)#1	119.3(4)
C(10)-C(11)-C(6)	118.2(2)	C(45)#1-C(45)-C(46)	120.3(2)
C(10)-C(11)-C(14)	120.4(2)	C(45)-C(46)-C(47)	118.7(3)
C(6)-C(11)-C(14)	121.3(2)	C(47)#1-C(47)-C(46)	121.0(2)
C(16)-C(15)-C(20)	122.4(2)		

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+3/2

Table 43. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(SIMes)(PPh_3)(CO)_2HF$ **(34)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	23(1)	16(1)	19(1)	1(1)	2(1)	0(1)
P(1)	22(1)	17(1)	21(1)	1(1)	2(1)	-1(1)
F(1)	47(1)	22(1)	25(1)	-3(1)	3(1)	-2(1)
O(1)	32(1)	68(1)	70(2)	33(1)	8(1)	15(1)
O(2)	59(1)	30(1)	36(1)	-11(1)	-2(1)	3(1)
N(1)	24(1)	21(1)	23(1)	6(1)	3(1)	3(1)
N(2)	23(1)	27(1)	25(1)	8(1)	3(1)	2(1)
C(1)	31(1)	32(1)	31(1)	10(1)	5(1)	-3(1)
C(2)	30(1)	23(1)	27(1)	3(1)	1(1)	2(1)
C(3)	24(1)	17(1)	19(1)	-1(1)	-1(1)	-2(1)
C(4)	27(1)	27(1)	27(1)	9(1)	2(1)	3(1)
C(5)	28(1)	35(1)	33(1)	16(1)	5(1)	3(1)
C(6)	28(1)	21(1)	21(1)	5(1)	5(1)	5(1)
C(7)	36(1)	23(1)	24(1)	5(1)	2(1)	8(1)
C(8)	44(2)	33(1)	24(1)	5(1)	8(1)	17(1)
C(9)	30(1)	46(2)	31(1)	14(1)	8(1)	15(1)
C(10)	26(1)	39(1)	34(1)	9(1)	1(1)	2(1)
C(11)	27(1)	29(1)	25(1)	5(1)	1(1)	4(1)
C(12)	48(2)	28(1)	31(1)	-4(1)	1(1)	5(1)
C(13)	38(2)	75(2)	46(2)	19(2)	16(1)	21(2)
C(14)	35(1)	35(1)	35(1)	-3(1)	1(1)	-3(1)
C(15)	22(1)	29(1)	27(1)	7(1)	2(1)	0(1)
C(16)	29(1)	38(1)	29(1)	6(1)	4(1)	2(1)

C(17)	32(1)	47(2)	41(2)	4(1)	10(1)	11(1)
C(18)	26(1)	55(2)	41(2)	13(1)	2(1)	6(1)
C(19)	26(1)	49(2)	37(1)	10(1)	-4(1)	-6(1)
C(20)	28(1)	31(1)	29(1)	7(1)	3(1)	-4(1)
C(21)	40(2)	50(2)	38(1)	-8(1)	3(1)	4(1)
C(22)	30(2)	89(3)	70(2)	5(2)	-3(2)	16(2)
C(23)	40(2)	35(1)	42(2)	-1(1)	-4(1)	-4(1)
C(24)	23(1)	20(1)	23(1)	-3(1)	2(1)	-1(1)
C(25)	27(1)	28(1)	30(1)	2(1)	3(1)	-1(1)
C(26)	25(1)	32(1)	40(1)	-1(1)	2(1)	6(1)
C(27)	24(1)	43(1)	32(1)	-10(1)	3(1)	5(1)
C(28)	35(1)	56(2)	21(1)	0(1)	5(1)	8(1)
C(29)	36(1)	36(1)	25(1)	2(1)	2(1)	9(1)
C(30)	28(1)	19(1)	19(1)	2(1)	-2(1)	-2(1)
C(31)	28(1)	27(1)	24(1)	1(1)	0(1)	-3(1)
C(32)	37(1)	29(1)	30(1)	4(1)	-1(1)	-13(1)
C(33)	54(2)	19(1)	30(1)	2(1)	-5(1)	-8(1)
C(34)	46(2)	24(1)	31(1)	-3(1)	4(1)	5(1)
C(35)	33(1)	21(1)	29(1)	1(1)	7(1)	0(1)
C(36)	21(1)	25(1)	23(1)	2(1)	3(1)	-1(1)
C(37)	27(1)	29(1)	27(1)	5(1)	1(1)	-4(1)
C(38)	32(1)	38(1)	32(1)	12(1)	0(1)	2(1)
C(39)	25(1)	52(2)	32(1)	3(1)	-6(1)	0(1)
C(40)	35(2)	38(1)	44(2)	-5(1)	-11(1)	-5(1)
C(41)	35(1)	26(1)	38(1)	1(1)	-6(1)	-1(1)
C(42)	80(3)	104(4)	88(3)	-16(3)	37(3)	-15(3)
C(43)	59(3)	82(3)	102(3)	1(3)	22(2)	-4(2)
C(44)	73(3)	79(3)	87(3)	12(2)	13(2)	2(2)
C(45)	70(2)	53(2)	57(2)	-10(2)	-3(2)	18(2)
C(46)	47(2)	94(3)	55(2)	-8(2)	11(2)	-9(2)
C(47)	102(3)	54(2)	40(2)	6(2)	-3(2)	-30(2)

Table 44. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIMes)(PPh_3)$(CO)_2$HF **(34)**.

Atom	x	y	z	U(eq)
H(4A)	1649	60	7361	33
H(4B)	1515	-713	6540	33
H(5A)	1046	-261	6869	38
H(5B)	1181	553	7645	38
H(8)	2247	-589	3949	40
H(10)	2558	1491	5867	40
H(12A)	1499	-316	4188	54
H(12B)	1610	-1171	4937	54
H(12C)	1738	-1109	3856	54
H(13A)	2743	23	3796	79
H(13B)	2901	89	4897	79
H(13C)	2826	1068	4277	79
H(14A)	1949	2440	6541	52
H(14B)	2262	2109	7104	52
H(14C)	1955	1560	7325	52
H(17)	336	2933	6865	47
H(19)	201	931	4692	45
H(21A)	943	2211	8009	64

H(21B)	824	3256	7618	64
H(21C)	1114	2771	7166	64
H(22A)	-239	1797	5791	95
H(22B)	-149	2450	4871	95
H(22C)	-136	2909	5965	95
H(23A)	857	-354	5093	59
H(23B)	895	430	4228	59
H(23C)	585	-164	4274	59
H(25)	1947	1665	3457	34
H(26)	2323	979	2544	39
H(27)	2422	1611	997	39
H(28)	2140	2928	345	45
H(29)	1749	3578	1211	39
H(31)	2025	4493	2741	32
H(32)	2126	6157	2992	39
H(33)	1789	7140	3787	41
H(34)	1352	6464	4363	40
H(35)	1245	4808	4106	33
H(37)	1245	4858	1896	33
H(38)	882	4962	564	41
H(39)	634	3558	-40	44
H(40)	738	2049	725	48
H(41)	1095	1941	2077	40
H(42)	233	5207	6024	107
H(43)	524	5228	7518	96
H(44)	291	5230	9001	95
H(45)	254	7516	7391	72
H(46)	512	8987	7269	78
H(47)	244	10460	7355	79
H(1)	1815	2232	4686	27(6)

Table 45. Crystal data and structure refinement for Ru(SIMes)(PPh_3)(COHF **(39)**.

Compound	Ru(SIMes)(PPh_3)(COHF **(39)**.
Empirical formula	C58 H58 N2 O P2 Ru
Formula weight	962.07
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.3050(2)Å α = 96.212(1)^o
	b = 11.8970(3)Å β = 96.477(1)^o
	c = 20.7740(6)Å γ = 118.000(2)^o
Volume	2409.50(10) Å^3
Z	2
Density (calculated)	1.326 Mg/m^3
Absorption coefficient	0.435 mm^{-1}
F(000)	1004
Crystal size	0.25 x 0.13 x 0.10 mm
Theta range for data collection	3.62 to 27.45^o
Index ranges	-14<=h<=14; -15<=k<=15; -25<=l<=26
Reflections collected	24476
Independent reflections	10596 [R(int) = 0.0441]
Reflections observed (>2σ)	8742
Data Completeness	0.961
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.96 and 0.92
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10596 / 2 / 601
Goodness-of-fit on F^2	1.146
Final R indices [I>2σ(I)]	R^1 = 0.0504 wR_2 = 0.1100
R indices (all data)	R^1 = 0.0670 wR_2 = 0.1168
Largest diff. peak and hole	0.961 and -0.845 eÅ^{-3}

Table 46. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Ru(SIMes)(PPh_3)(COHF **(39)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	1073(1)	2606(1)	2189(1)	18(1)
P(1)	518(1)	525(1)	2317(1)	20(1)
P(2)	1693(1)	3691(1)	3295(1)	20(1)
O(1)	-1925(3)	1949(3)	1900(1)	34(1)
N(1)	3301(3)	4766(3)	1598(2)	24(1)
N(2)	1272(3)	4244(3)	1105(2)	25(1)
C(1)	-776(3)	2248(3)	1992(2)	23(1)
C(2)	1955(3)	4042(3)	1623(2)	21(1)
C(3)	3536(14)	5494(15)	1063(8)	29(3)
C(4)	2142(11)	5064(11)	674(6)	26(2)
C(5)	4486(3)	4848(3)	1984(2)	23(1)
C(6)	4846(3)	3879(3)	1832(2)	26(1)
C(7)	6038(4)	4030(4)	2186(2)	29(1)
C(8)	6912(4)	5125(4)	2666(2)	32(1)
C(9)	6569(4)	6090(4)	2775(2)	29(1)
C(10)	5373(3)	5983(3)	2436(2)	25(1)

C(11)	5110(4)	7126(4)	2534(2)	35(1)
C(12)	3991(4)	2721(4)	1290(2)	31(1)
C(13)	8215(4)	5257(5)	3043(3)	46(1)
C(14)	-161(3)	3585(3)	846(2)	24(1)
C(15)	-946(4)	4162(3)	1004(2)	26(1)
C(16)	-2323(4)	3529(4)	718(2)	28(1)
C(17)	-2925(3)	2367(4)	274(2)	28(1)
C(18)	-2107(4)	1839(4)	110(2)	28(1)
C(19)	-716(4)	2445(3)	377(2)	25(1)
C(20)	153(4)	1909(4)	128(2)	32(1)
C(21)	-320(4)	5467(4)	1445(2)	38(1)
C(22)	-4411(4)	1720(4)	-38(2)	38(1)
C(23)	-916(3)	-768(3)	1694(2)	21(1)
C(24)	-1416(3)	-494(3)	1125(2)	24(1)
C(25)	-2448(3)	-1455(3)	644(2)	27(1)
C(26)	-3019(3)	-2737(3)	734(2)	27(1)
C(27)	-2565(4)	-3031(3)	1299(2)	28(1)
C(28)	-1517(3)	-2062(3)	1780(2)	25(1)
C(29)	1920(3)	166(3)	2219(2)	22(1)
C(30)	1791(4)	-815(3)	1735(2)	27(1)
C(31)	2906(4)	-996(4)	1666(2)	34(1)
C(32)	4146(4)	-215(4)	2079(2)	34(1)
C(33)	4289(4)	756(4)	2566(2)	33(1)
C(34)	3178(4)	943(3)	2628(2)	27(1)
C(35)	-7(3)	-128(3)	3067(2)	23(1)
C(36)	640(4)	-649(4)	3440(2)	31(1)
C(37)	203(5)	-1090(4)	4012(2)	39(1)
C(38)	-869(5)	-1001(4)	4211(2)	40(1)
C(39)	-1525(5)	-492(4)	3844(2)	40(1)
C(40)	-1101(4)	-57(4)	3276(2)	31(1)
C(41)	2959(3)	3409(3)	3780(2)	22(1)
C(42)	4313(4)	4054(4)	3701(2)	29(1)
C(43)	5261(4)	3750(4)	4000(2)	33(1)
C(44)	4856(4)	2769(4)	4371(2)	34(1)
C(45)	3520(4)	2124(4)	4447(2)	31(1)
C(46)	2575(4)	2440(3)	4160(2)	26(1)
C(47)	459(3)	3390(3)	3862(2)	23(1)
C(48)	892(4)	3800(4)	4541(2)	30(1)
C(49)	-42(4)	3576(4)	4957(2)	34(1)
C(50)	-1420(4)	2956(4)	4702(2)	37(1)
C(51)	-1860(4)	2583(4)	4035(2)	37(1)
C(52)	-935(4)	2782(4)	3611(2)	30(1)
C(53)	2450(4)	5465(3)	3444(2)	25(1)
C(54)	1826(4)	5960(3)	3031(2)	29(1)
C(55)	2241(4)	7271(4)	3121(2)	33(1)
C(56)	3312(4)	8123(4)	3627(2)	33(1)
C(57)	3948(4)	7658(3)	4042(2)	33(1)
C(58)	3522(4)	6336(3)	3955(2)	30(1)
C(3A)	3590(20)	5320(20)	965(12)	21(5)
C(4A)	2154(18)	5306(16)	787(8)	17(4)

Table 47. Bond lengths [Å] and angles [°] for Ru(SIMes)(PPh_3)(COHF **(39)**.

Ru(1)-H(2)	1.592(10)	C(19)-C(20)	1.508(5)
Ru(1)-H(1)	1.604(10)	C(23)-C(24)	1.389(5)
Ru(1)-C(1)	1.910(3)	C(23)-C(28)	1.403(4)
Ru(1)-C(2)	2.097(3)	C(24)-C(25)	1.380(5)
Ru(1)-P(1)	2.3058(8)	C(25)-C(26)	1.393(5)
Ru(1)-P(2)	2.3622(10)	C(26)-C(27)	1.374(5)
P(1)-C(35)	1.849(3)	C(27)-C(28)	1.390(5)
P(1)-C(29)	1.850(3)	C(29)-C(34)	1.387(5)
P(1)-C(23)	1.850(4)	C(29)-C(30)	1.396(5)
P(2)-C(41)	1.838(3)	C(30)-C(31)	1.394(5)
P(2)-C(53)	1.840(3)	C(31)-C(32)	1.378(6)
P(2)-C(47)	1.859(3)	C(32)-C(33)	1.385(6)
O(1)-C(1)	1.160(4)	C(33)-C(34)	1.392(5)
N(1)-C(2)	1.362(4)	C(35)-C(36)	1.386(5)
N(1)-C(5)	1.438(4)	C(35)-C(40)	1.392(5)
N(1)-C(3)	1.453(15)	C(36)-C(37)	1.399(5)
N(1)-C(3A)	1.53(2)	C(37)-C(38)	1.369(6)
N(2)-C(2)	1.362(4)	C(38)-C(39)	1.375(6)
N(2)-C(14)	1.431(4)	C(39)-C(40)	1.385(6)
N(2)-C(4A)	1.473(18)	C(41)-C(42)	1.393(5)
N(2)-C(4)	1.485(11)	C(41)-C(46)	1.393(5)
C(3)-C(4)	1.505(19)	C(42)-C(43)	1.388(5)
C(5)-C(10)	1.398(5)	C(43)-C(44)	1.393(6)
C(5)-C(6)	1.408(5)	C(44)-C(45)	1.373(5)
C(6)-C(7)	1.382(5)	C(45)-C(46)	1.386(5)
C(6)-C(12)	1.506(5)	C(47)-C(48)	1.393(5)
C(7)-C(8)	1.399(6)	C(47)-C(52)	1.393(5)
C(8)-C(9)	1.380(5)	C(48)-C(49)	1.386(5)
C(8)-C(13)	1.518(5)	C(49)-C(50)	1.379(6)
C(9)-C(10)	1.394(5)	C(50)-C(51)	1.366(6)
C(10)-C(11)	1.521(5)	C(51)-C(52)	1.394(5)
C(14)-C(15)	1.398(5)	C(53)-C(54)	1.395(5)
C(14)-C(19)	1.400(5)	C(53)-C(58)	1.401(5)
C(15)-C(16)	1.392(5)	C(54)-C(55)	1.385(5)
C(15)-C(21)	1.505(5)	C(55)-C(56)	1.388(6)
C(16)-C(17)	1.387(6)	C(56)-C(57)	1.379(6)
C(17)-C(18)	1.392(5)	C(57)-C(58)	1.396(5)
C(17)-C(22)	1.506(5)	C(3A)-C(4A)	1.62(3)
C(18)-C(19)	1.397(5)		
H(2)-Ru(1)-H(1)	80(2)	C(16)-C(15)-C(14)	118.4(3)
H(2)-Ru(1)-C(1)	176.7(14)	C(16)-C(15)-C(21)	120.0(3)
H(1)-Ru(1)-C(1)	99.7(16)	C(14)-C(15)-C(21)	121.5(3)
H(2)-Ru(1)-C(2)	83.4(14)	C(17)-C(16)-C(15)	122.1(3)
H(1)-Ru(1)-C(2)	74.6(16)	C(16)-C(17)-C(18)	118.1(3)
C(1)-Ru(1)-C(2)	99.56(13)	C(16)-C(17)-C(22)	120.9(3)
H(2)-Ru(1)-P(1)	82.0(14)	C(18)-C(17)-C(22)	121.0(4)
H(1)-Ru(1)-P(1)	72.1(16)	C(17)-C(18)-C(19)	122.0(4)
C(1)-Ru(1)-P(1)	94.71(10)	C(18)-C(19)-C(14)	118.1(3)
C(2)-Ru(1)-P(1)	145.49(9)	C(18)-C(19)-C(20)	119.7(3)
H(2)-Ru(1)-P(2)	80.2(15)	C(14)-C(19)-C(20)	122.0(3)
H(1)-Ru(1)-P(2)	159.4(16)	C(24)-C(23)-C(28)	118.0(3)
C(1)-Ru(1)-P(2)	100.36(11)	C(24)-C(23)-P(1)	121.3(2)

C(2)-Ru(1)-P(2)	106.30(10)	C(28)-C(23)-P(1)	120.7(3)
P(1)-Ru(1)-P(2)	101.74(3)	C(25)-C(24)-C(23)	121.9(3)
C(35)-P(1)-C(29)	101.85(15)	C(24)-C(25)-C(26)	119.3(3)
C(35)-P(1)-C(23)	98.91(15)	C(27)-C(26)-C(25)	120.0(3)
C(29)-P(1)-C(23)	102.29(16)	C(26)-C(27)-C(28)	120.6(3)
C(35)-P(1)-Ru(1)	123.63(11)	C(27)-C(28)-C(23)	120.2(3)
C(29)-P(1)-Ru(1)	112.32(11)	C(34)-C(29)-C(30)	118.2(3)
C(23)-P(1)-Ru(1)	114.92(11)	C(34)-C(29)-P(1)	118.5(3)
C(41)-P(2)-C(53)	104.03(16)	C(30)-C(29)-P(1)	123.2(3)
C(41)-P(2)-C(47)	100.40(15)	C(31)-C(30)-C(29)	120.5(4)
C(53)-P(2)-C(47)	96.35(15)	C(32)-C(31)-C(30)	120.3(4)
C(41)-P(2)-Ru(1)	111.95(11)	C(31)-C(32)-C(33)	120.0(3)
C(53)-P(2)-Ru(1)	117.55(12)	C(32)-C(33)-C(34)	119.5(4)
C(47)-P(2)-Ru(1)	123.49(12)	C(29)-C(34)-C(33)	121.5(3)
C(2)-N(1)-C(5)	130.2(3)	C(36)-C(35)-C(40)	118.3(3)
C(2)-N(1)-C(3)	113.3(6)	C(36)-C(35)-P(1)	124.3(3)
C(5)-N(1)-C(3)	116.3(6)	C(40)-C(35)-P(1)	117.4(3)
C(2)-N(1)-C(3A)	115.1(9)	C(35)-C(36)-C(37)	120.8(4)
C(5)-N(1)-C(3A)	112.8(9)	C(38)-C(37)-C(36)	119.9(4)
C(3)-N(1)-C(3A)	11.5(12)	C(37)-C(38)-C(39)	120.1(4)
C(2)-N(2)-C(14)	128.7(3)	C(38)-C(39)-C(40)	120.4(4)
C(2)-N(2)-C(4A)	114.0(7)	C(39)-C(40)-C(35)	120.6(4)
C(14)-N(2)-C(4A)	117.3(7)	C(42)-C(41)-C(46)	118.4(3)
C(2)-N(2)-C(4)	115.1(5)	C(42)-C(41)-P(2)	119.4(3)
C(14)-N(2)-C(4)	115.0(5)	C(46)-C(41)-P(2)	121.6(3)
C(4A)-N(2)-C(4)	13.4(8)	C(43)-C(42)-C(41)	120.8(3)
O(1)-C(1)-Ru(1)	174.4(3)	C(42)-C(43)-C(44)	120.0(3)
N(2)-C(2)-N(1)	105.3(3)	C(45)-C(44)-C(43)	119.4(3)
N(2)-C(2)-Ru(1)	125.5(2)	C(44)-C(45)-C(46)	120.8(3)
N(1)-C(2)-Ru(1)	127.9(2)	C(45)-C(46)-C(41)	120.5(3)
N(1)-C(3)-C(4)	105.4(9)	C(48)-C(47)-C(52)	118.0(3)
N(2)-C(4)-C(3)	100.4(8)	C(48)-C(47)-P(2)	121.6(3)
C(10)-C(5)-C(6)	120.7(3)	C(52)-C(47)-P(2)	120.3(3)
C(10)-C(5)-N(1)	119.0(3)	C(49)-C(48)-C(47)	120.9(4)
C(6)-C(5)-N(1)	119.6(3)	C(50)-C(49)-C(48)	120.4(4)
C(7)-C(6)-C(5)	118.1(3)	C(51)-C(50)-C(49)	119.5(4)
C(7)-C(6)-C(12)	120.0(3)	C(50)-C(51)-C(52)	120.8(4)
C(5)-C(6)-C(12)	121.9(3)	C(47)-C(52)-C(51)	120.4(4)
C(6)-C(7)-C(8)	122.3(3)	C(54)-C(53)-C(58)	118.0(3)
C(9)-C(8)-C(7)	118.0(3)	C(54)-C(53)-P(2)	115.9(3)
C(9)-C(8)-C(13)	121.2(4)	C(58)-C(53)-P(2)	126.0(3)
C(7)-C(8)-C(13)	120.8(4)	C(55)-C(54)-C(53)	121.5(4)
C(8)-C(9)-C(10)	122.0(4)	C(54)-C(55)-C(56)	119.8(3)
C(9)-C(10)-C(5)	118.6(3)	C(57)-C(56)-C(55)	119.9(3)
C(9)-C(10)-C(11)	119.5(3)	C(56)-C(57)-C(58)	120.3(4)
C(5)-C(10)-C(11)	121.7(3)	C(57)-C(58)-C(53)	120.5(3)
C(15)-C(14)-C(19)	121.1(3)	N(1)-C(3A)-C(4A)	95.7(13)
C(15)-C(14)-N(2)	119.8(3)	N(2)-C(4A)-C(3A)	100.9(13)
C(19)-C(14)-N(2)	118.7(3)		

Table 48. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIMes)(PPh_3)(COHF **(39)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	18(1)	17(1)	21(1)	6(1)	4(1)	9(1)
P(1)	21(1)	18(1)	22(1)	6(1)	3(1)	10(1)
P(2)	22(1)	18(1)	22(1)	6(1)	4(1)	11(1)
O(1)	25(1)	45(2)	37(2)	15(1)	6(1)	19(1)
N(1)	18(1)	22(1)	29(2)	12(1)	5(1)	7(1)
N(2)	22(1)	26(2)	29(2)	14(1)	6(1)	10(1)
C(1)	25(2)	24(2)	26(2)	10(1)	8(1)	15(2)
C(2)	22(2)	18(2)	24(2)	4(1)	4(1)	10(1)
C(3)	28(4)	34(6)	31(7)	15(5)	14(4)	16(4)
C(4)	32(4)	21(5)	28(5)	11(4)	11(4)	13(4)
C(5)	17(2)	24(2)	26(2)	9(1)	4(1)	8(1)
C(6)	22(2)	23(2)	31(2)	8(2)	10(1)	8(1)
C(7)	24(2)	28(2)	39(2)	15(2)	12(2)	14(2)
C(8)	25(2)	37(2)	32(2)	16(2)	6(2)	12(2)
C(9)	24(2)	29(2)	27(2)	7(2)	5(2)	6(2)
C(10)	22(2)	25(2)	29(2)	8(2)	8(1)	10(1)
C(11)	32(2)	25(2)	45(3)	5(2)	13(2)	11(2)
C(12)	29(2)	28(2)	35(2)	3(2)	8(2)	14(2)
C(13)	29(2)	61(3)	47(3)	24(2)	4(2)	19(2)
C(14)	23(2)	28(2)	24(2)	12(1)	4(1)	14(2)
C(15)	30(2)	28(2)	26(2)	11(2)	7(2)	17(2)
C(16)	29(2)	34(2)	32(2)	13(2)	9(2)	22(2)
C(17)	22(2)	30(2)	34(2)	14(2)	6(2)	13(2)
C(18)	27(2)	27(2)	28(2)	8(2)	4(2)	12(2)
C(19)	26(2)	31(2)	26(2)	13(2)	7(1)	17(2)
C(20)	35(2)	41(2)	30(2)	10(2)	8(2)	25(2)
C(21)	40(2)	38(2)	40(3)	3(2)	-2(2)	25(2)
C(22)	27(2)	42(2)	48(3)	12(2)	4(2)	19(2)
C(23)	21(2)	20(2)	24(2)	6(1)	4(1)	10(1)
C(24)	21(2)	23(2)	30(2)	6(1)	3(1)	12(1)
C(25)	25(2)	31(2)	27(2)	5(2)	2(1)	16(2)
C(26)	17(2)	24(2)	32(2)	-1(2)	3(1)	5(1)
C(27)	25(2)	20(2)	36(2)	6(2)	9(2)	8(1)
C(28)	23(2)	21(2)	29(2)	8(1)	6(1)	9(1)
C(29)	29(2)	22(2)	24(2)	9(1)	7(1)	16(1)
C(30)	30(2)	22(2)	31(2)	4(2)	4(2)	15(2)
C(31)	39(2)	34(2)	36(2)	6(2)	10(2)	23(2)
C(32)	35(2)	37(2)	46(3)	14(2)	12(2)	27(2)
C(33)	28(2)	32(2)	41(2)	8(2)	0(2)	18(2)
C(34)	29(2)	24(2)	33(2)	4(2)	4(2)	17(2)
C(35)	27(2)	16(2)	23(2)	6(1)	4(1)	8(1)
C(36)	40(2)	28(2)	27(2)	9(2)	6(2)	17(2)
C(37)	51(2)	32(2)	30(2)	14(2)	2(2)	18(2)
C(38)	55(3)	32(2)	27(2)	10(2)	12(2)	13(2)
C(39)	45(2)	37(2)	35(2)	8(2)	19(2)	15(2)
C(40)	33(2)	27(2)	34(2)	8(2)	10(2)	14(2)
C(41)	24(2)	22(2)	19(2)	3(1)	2(1)	12(1)
C(42)	27(2)	32(2)	27(2)	8(2)	4(2)	13(2)
C(43)	26(2)	44(2)	30(2)	8(2)	5(2)	18(2)

C(44)	35(2)	49(2)	30(2)	10(2)	3(2)	30(2)
C(45)	37(2)	35(2)	29(2)	12(2)	5(2)	22(2)
C(46)	29(2)	27(2)	25(2)	7(2)	6(2)	15(2)
C(47)	28(2)	20(2)	28(2)	8(1)	8(1)	15(1)
C(48)	33(2)	31(2)	29(2)	8(2)	7(2)	17(2)
C(49)	47(2)	39(2)	26(2)	8(2)	13(2)	28(2)
C(50)	41(2)	44(2)	41(3)	17(2)	23(2)	27(2)
C(51)	27(2)	44(2)	43(3)	11(2)	13(2)	17(2)
C(52)	33(2)	35(2)	29(2)	9(2)	9(2)	21(2)
C(53)	30(2)	21(2)	25(2)	6(1)	7(1)	13(2)
C(54)	30(2)	25(2)	32(2)	3(2)	0(2)	15(2)
C(55)	42(2)	31(2)	38(2)	11(2)	7(2)	26(2)
C(56)	45(2)	21(2)	37(2)	5(2)	10(2)	18(2)
C(57)	39(2)	21(2)	30(2)	2(2)	5(2)	9(2)
C(58)	37(2)	23(2)	26(2)	7(2)	2(2)	13(2)

Table 49. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIMes)(PPh_3)(COHF **(39)**.

Atom	x	y	z	U(eq)
H(3A)	4095	5299	783	35
H(3B)	4013	6436	1238	35
H(4A)	1990	5808	626	31
H(4B)	1990	4559	233	31
H(7)	6273	3367	2099	34
H(9)	7165	6851	3090	35
H(11A)	5596	7738	2254	52
H(11B)	5434	7559	2997	52
H(11C)	4129	6817	2415	52
H(12A)	4437	2190	1245	46
H(12B)	3889	3013	875	46
H(12C)	3089	2206	1399	46
H(13A)	8973	6124	3053	69
H(13B)	8409	4605	2825	69
H(13C)	8104	5126	3495	69
H(16)	-2868	3905	831	34
H(18)	-2505	1044	-194	34
H(20A)	685	2442	-172	48
H(20B)	-433	1017	-109	48
H(20C)	774	1921	501	48
H(21A)	-393	6090	1194	57
H(21B)	643	5762	1614	57
H(21C)	-802	5400	1815	57
H(22A)	-4959	1136	239	57
H(22B)	-4555	1222	-475	57
H(22C)	-4686	2380	-82	57
H(24)	-1037	381	1065	29
H(25)	-2764	-1245	256	33
H(26)	-3724	-3407	404	32
H(27)	-2970	-3905	1362	33
H(28)	-1206	-2277	2168	30
H(30)	938	-1363	1451	33
H(31)	2810	-1661	1332	40
H(32)	4902	-343	2031	41

H(33)	5139	1290	2856	39
H(34)	3285	1619	2958	33
H(36)	1388	-708	3305	38
H(37)	650	-1451	4263	46
H(38)	-1160	-1291	4602	48
H(39)	-2273	-438	3982	48
H(40)	-1562	293	3026	38
H(42)	4591	4710	3440	34
H(43)	6186	4212	3951	40
H(44)	5498	2548	4570	41
H(45)	3241	1454	4699	38
H(46)	1657	1993	4222	31
H(48)	1839	4238	4722	36
H(49)	269	3852	5420	41
H(50)	-2059	2790	4988	45
H(51)	-2807	2182	3858	45
H(52)	-1258	2501	3150	36
H(54)	1101	5386	2680	35
H(55)	1794	7587	2838	40
H(56)	3605	9024	3688	40
H(57)	4680	8241	4388	39
H(58)	3962	6024	4245	35
H(3A1)	3706	4742	626	25
H(3A2)	4384	6200	1047	25
H(4A1)	2221	6139	977	20
H(4A2)	1827	5116	305	20
H(1)	1150(40)	1870(40)	1516(12)	46(13)
H(2)	2582(17)	2820(40)	2360(20)	31(11)

Table 50. Crystal data and structure refinement for $Ru(IPr)(PPH_3)(CO)_2HF$ **(45)**.

Compound	$Ru(IPr)(PPH_3)(CO)_2HF$ **(45)**
Empirical formula	C49 H52 F N2 O3 P Ru
Formula weight	867.97
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P212121
Unit cell dimensions	a = 10.7450(1)Å α = 90°
	b = 31.7660(3)Å β= 90°
	c = 12.5000(1)Å γ = 90°
Volume	4266.57(7) Å3
Z	4
Density (calculated)	1.351 Mg/m^3
Absorption coefficient	0.453 mm^{-1}
F(000)	1808
Crystal size	0.25 x 0.25 x 0.15 mm
Theta range for data collection	3.58 to 30.05°
Index ranges	-15<=h<=15; -44<=k<=44; -17<=l<=17
Reflections collected	59628
Independent reflections	12460 [R(int) = 0.0842]
Reflections observed (>2σ)	11277
Data Completeness	0.996
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.94 and 0.88
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12460 / 8 / 523
Goodness-of-fit on F2	1.076
Final R indices [I>2σ(I)]	R1 = 0.0450 wR2 = 0.0978
R indices (all data)	R1 = 0.0523 wR2 = 0.1012
Absolute structure parameter	0.21(2)
Largest diff. peak and hole	0.838 and -0.866 $eÅ^{-3}$

Table 51. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IPr)(PPH_3)(CO)_2HF$ **(45)**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	6195(1)	1390(1)	8374(1)	23(1)
P(1)	6794(1)	1569(1)	6618(1)	21(1)
C(2A)	7865(3)	1389(2)	8863(4)	2(1)
F(1A)	4388(4)	1343(2)	7931(5)	28(1)
O(1)	5886(3)	2299(1)	9259(3)	51(1)
O(2)	3508(3)	1485(2)	7619(4)	44(1)
N(1)	5536(2)	1139(1)	10745(2)	24(1)
N(2)	5597(2)	598(1)	9725(2)	22(1)
C(1)	5997(3)	1962(1)	8988(3)	32(1)
C(2)	4540(5)	1440(4)	7897(13)	30(3)
C(3)	5704(3)	1027(1)	9705(2)	21(1)
C(4)	5347(3)	793(1)	11390(2)	27(1)
C(5)	5388(3)	454(1)	10753(3)	27(1)
C(6)	5361(3)	1564(1)	11139(3)	27(1)
C(7)	4155(3)	1732(1)	11097(3)	33(1)

C(8)	3976(4)	2126(1)	11561(4)	47(1)
C(9)	4952(4)	2340(1)	12036(4)	52(1)
C(10)	6140(4)	2169(1)	12046(3)	45(1)
C(11)	6376(3)	1777(1)	11600(3)	32(1)
C(12)	3072(3)	1500(1)	10587(3)	39(1)
C(13)	2266(4)	1782(2)	9884(4)	57(1)
C(14)	2274(4)	1283(2)	11429(4)	61(1)
C(15)	7679(3)	1591(1)	11612(4)	36(1)
C(16)	8660(4)	1912(1)	11256(4)	53(1)
C(17)	7988(4)	1425(2)	12728(3)	46(1)
C(18)	5556(3)	308(1)	8832(2)	23(1)
C(19)	6664(3)	122(1)	8472(3)	28(1)
C(20)	6570(4)	-185(1)	7687(3)	36(1)
C(21)	5421(4)	-299(1)	7268(3)	42(1)
C(22)	4359(4)	-104(1)	7614(3)	36(1)
C(23)	8411(4)	-87(1)	9681(4)	48(1)
C(24)	4393(3)	207(1)	8409(3)	27(1)
C(25)	7913(3)	248(1)	8925(3)	32(1)
C(27)	8865(4)	338(1)	8030(4)	49(1)
C(28)	3206(3)	422(1)	8773(3)	33(1)
C(29)	2481(4)	141(2)	9532(4)	52(1)
C(30)	2383(4)	558(2)	7840(4)	51(1)
C(31)	8296(3)	1347(1)	6218(2)	24(1)
C(32)	9363(3)	1470(1)	6759(3)	36(1)
C(33)	10511(3)	1310(1)	6479(4)	42(1)
C(34)	10599(3)	1013(1)	5680(3)	42(1)
C(35)	9553(3)	885(1)	5136(3)	42(1)
C(36)	8407(3)	1050(1)	5399(3)	32(1)
C(37)	5686(3)	1359(1)	5641(2)	24(1)
C(38)	5105(3)	975(1)	5844(3)	31(1)
C(39)	4239(3)	815(1)	5138(3)	37(1)
C(40)	3938(3)	1032(1)	4221(3)	40(1)
C(41)	4514(3)	1412(2)	3995(3)	38(1)
C(42)	5392(3)	1577(1)	4709(3)	30(1)
C(43)	6920(3)	2120(1)	6199(3)	25(1)
C(44)	7837(3)	2261(1)	5505(3)	34(1)
C(45)	7824(4)	2675(1)	5144(4)	45(1)
C(46)	6914(4)	2948(1)	5479(4)	45(1)
C(47)	5993(4)	2814(1)	6177(3)	41(1)
C(48)	5994(2)	2395(1)	6542(2)	32(1)
O(2A)	8883(2)	1363(1)	9158(2)	44(1)
O(3B)	9651(2)	1017(1)	9854(2)	43(1)
O(3A)	3281(2)	1905(1)	7171(2)	49(2)
F(1)	7982(4)	1263(1)	8833(4)	44(1)

Table 52. Bond lengths [Å] and angles [°] for Ru(IPr)(PPH_3)($CO)_2$HF **(45)**.

Ru(1)-C(2)	1.883(3)	Ru(1)-C(2A)	1.896(2)
Ru(1)-C(1)	1.983(3)	Ru(1)-F(1A)	2.025(4)
Ru(1)-F(1)	2.044(4)	Ru(1)-C(3)	2.092(3)
Ru(1)-P(1)	2.3572(9)	P(1)-C(31)	1.831(3)
P(1)-C(37)	1.832(3)	P(1)-C(43)	1.833(3)
C(2A)-O(2A)	1.157(2)	O(1)-C(1)	1.128(4)
O(2)-C(2)	1.171(3)	N(1)-C(3)	1.360(4)
N(1)-C(4)	1.378(4)	N(1)-C(6)	1.449(4)

N(2)-C(3)	1.367(4)	N(2)-C(5)	1.383(4)
N(2)-C(18)	1.448(4)	C(4)-C(5)	1.341(4)
C(6)-C(7)	1.402(5)	C(6)-C(11)	1.408(5)
C(7)-C(8)	1.393(5)	C(7)-C(12)	1.517(5)
C(8)-C(9)	1.384(6)	C(9)-C(10)	1.387(6)
C(10)-C(11)	1.387(5)	C(11)-C(15)	1.521(5)
C(12)-C(14)	1.523(6)	C(12)-C(13)	1.524(6)
C(15)-C(17)	1.527(6)	C(15)-C(16)	1.532(5)
C(18)-C(24)	1.394(4)	C(18)-C(19)	1.403(4)
C(19)-C(20)	1.389(5)	C(19)-C(25)	1.511(5)
C(20)-C(21)	1.388(6)	C(21)-C(22)	1.369(6)
C(22)-C(24)	1.401(5)	C(23)-C(25)	1.521(5)
C(24)-C(28)	1.517(5)	C(25)-C(27)	1.542(5)
C(28)-C(29)	1.517(5)	C(28)-C(30)	1.527(5)
C(31)-C(32)	1.387(4)	C(31)-C(36)	1.396(5)
C(32)-C(33)	1.380(5)	C(33)-C(34)	1.376(6)
C(34)-C(35)	1.375(6)	C(35)-C(36)	1.379(5)
C(37)-C(42)	1.391(4)	C(37)-C(38)	1.394(4)
C(38)-C(39)	1.379(5)	C(39)-C(40)	1.376(6)
C(40)-C(41)	1.386(6)	C(41)-C(42)	1.400(5)
C(43)-C(44)	1.386(5)	C(43)-C(48)	1.391(4)
C(44)-C(45)	1.390(5)	C(45)-C(46)	1.373(6)
C(46)-C(47)	1.387(6)	C(47)-C(48)	1.406(4)
C(2)-Ru(1)-C(2A)	175.3(4)	C(2)-Ru(1)-C(1)	86.8(4)
C(2A)-Ru(1)-C(1)	88.8(2)	C(2)-Ru(1)-F(1A)	9.4(5)
C(2A)-Ru(1)-F(1A)	174.8(2)	C(1)-Ru(1)-F(1A)	94.0(2)
C(2)-Ru(1)-F(1)	173.1(4)	C(2A)-Ru(1)-F(1)	11.5(2)
C(1)-Ru(1)-F(1)	100.01(16)	F(1A)-Ru(1)-F(1)	164.3(2)
C(2)-Ru(1)-C(3)	93.4(5)	C(2A)-Ru(1)-C(3)	88.90(19)
C(1)-Ru(1)-C(3)	99.80(12)	F(1A)-Ru(1)-C(3)	86.3(2)
F(1)-Ru(1)-C(3)	84.52(17)	C(2)-Ru(1)-P(1)	86.7(5)
C(2A)-Ru(1)-P(1)	92.42(17)	C(1)-Ru(1)-P(1)	99.70(10)
F(1A)-Ru(1)-P(1)	91.4(2)	F(1)-Ru(1)-P(1)	93.01(16)
C(3)-Ru(1)-P(1)	160.48(8)	C(31)-P(1)-C(37)	104.48(14)
C(31)-P(1)-C(43)	103.03(14)	C(37)-P(1)-C(43)	101.84(15)
C(31)-P(1)-Ru(1)	113.71(10)	C(37)-P(1)-Ru(1)	110.82(10)
C(43)-P(1)-Ru(1)	121.14(11)	O(2A)-C(2A)-Ru(1)	176.2(5)
C(3)-N(1)-C(4)	111.7(3)	C(3)-N(1)-C(6)	125.9(3)
C(4)-N(1)-C(6)	121.7(2)	C(3)-N(2)-C(5)	111.2(3)
C(3)-N(2)-C(18)	128.5(3)	C(5)-N(2)-C(18)	120.0(2)
O(1)-C(1)-Ru(1)	174.7(3)	O(2)-C(2)-Ru(1)	177.4(12)
N(1)-C(3)-N(2)	103.5(2)	N(1)-C(3)-Ru(1)	130.5(2)
N(2)-C(3)-Ru(1)	125.8(2)	C(5)-C(4)-N(1)	106.9(3)
C(4)-C(5)-N(2)	106.8(3)	C(7)-C(6)-C(11)	123.2(3)
C(7)-C(6)-N(1)	117.5(3)	C(11)-C(6)-N(1)	119.1(3)
C(8)-C(7)-C(6)	117.0(3)	C(8)-C(7)-C(12)	120.3(3)
C(6)-C(7)-C(12)	122.6(3)	C(9)-C(8)-C(7)	121.0(3)
C(8)-C(9)-C(10)	120.6(4)	C(11)-C(10)-C(9)	121.1(4)
C(10)-C(11)-C(6)	117.0(3)	C(10)-C(11)-C(15)	121.0(3)
C(6)-C(11)-C(15)	122.0(3)	C(7)-C(12)-C(14)	111.2(3)
C(7)-C(12)-C(13)	113.1(3)	C(14)-C(12)-C(13)	110.2(3)
C(11)-C(15)-C(17)	110.1(3)	C(11)-C(15)-C(16)	111.8(3)
C(17)-C(15)-C(16)	110.2(3)	C(24)-C(18)-C(19)	122.8(3)
C(24)-C(18)-N(2)	117.8(3)	C(19)-C(18)-N(2)	119.3(3)

C(20)-C(19)-C(18)	117.5(3)	C(20)-C(19)-C(25)	121.1(3)
C(18)-C(19)-C(25)	121.5(3)	C(21)-C(20)-C(19)	120.9(3)
C(22)-C(21)-C(20)	120.3(3)	C(21)-C(22)-C(24)	121.4(3)
C(18)-C(24)-C(22)	117.1(3)	C(18)-C(24)-C(28)	122.4(3)
C(22)-C(24)-C(28)	120.5(3)	C(19)-C(25)-C(23)	111.1(3)
C(19)-C(25)-C(27)	111.4(3)	C(23)-C(25)-C(27)	110.3(3)
C(24)-C(28)-C(29)	110.8(3)	C(24)-C(28)-C(30)	112.7(3)
C(29)-C(28)-C(30)	110.3(3)	C(32)-C(31)-C(36)	118.5(3)
C(32)-C(31)-P(1)	119.1(2)	C(36)-C(31)-P(1)	122.4(2)
C(33)-C(32)-C(31)	120.8(4)	C(34)-C(33)-C(32)	119.8(3)
C(35)-C(34)-C(33)	120.4(3)	C(34)-C(35)-C(36)	120.0(4)
C(35)-C(36)-C(31)	120.5(3)	C(42)-C(37)-C(38)	119.1(3)
C(42)-C(37)-P(1)	121.7(2)	C(38)-C(37)-P(1)	119.3(2)
C(39)-C(38)-C(37)	120.6(3)	C(40)-C(39)-C(38)	120.4(3)
C(39)-C(40)-C(41)	120.1(3)	C(40)-C(41)-C(42)	119.7(3)
C(37)-C(42)-C(41)	120.1(3)	C(44)-C(43)-C(48)	120.0(3)
C(44)-C(43)-P(1)	122.6(3)	C(48)-C(43)-P(1)	117.3(2)
C(43)-C(44)-C(45)	120.0(3)	C(46)-C(45)-C(44)	120.4(4)
C(45)-C(46)-C(47)	120.3(3)	C(46)-C(47)-C(48)	119.7(3)
C(43)-C(48)-C(47)	119.6(3)		

Table 53. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IPr)(PPH_3)(CO)_2HF$ **(45)**. The anisotropic displacement factor exponent takes the form: -2 gpi2 [h2 a*2 U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	28(1)	19(1)	21(1)	2(1)	2(1)	-1(1)
P(1)	22(1)	20(1)	22(1)	3(1)	-1(1)	-2(1)
F(1A)	16(2)	39(4)	29(2)	4(2)	-5(2)	-3(2)
O(1)	82(2)	26(1)	46(2)	-3(1)	0(2)	1(1)
O(2)	22(2)	68(4)	41(3)	10(3)	-4(2)	4(2)
N(1)	27(1)	23(1)	21(1)	1(1)	3(1)	2(1)
N(2)	25(1)	23(1)	16(1)	2(1)	1(1)	1(1)
C(1)	48(2)	20(1)	27(2)	-1(1)	-1(1)	-3(1)
C(3)	22(1)	20(1)	20(1)	2(1)	2(1)	2(1)
C(4)	35(2)	27(1)	21(2)	5(1)	1(1)	3(1)
C(5)	35(2)	25(1)	20(2)	6(1)	3(1)	2(1)
C(6)	36(2)	25(1)	20(2)	-2(1)	1(1)	5(1)
C(7)	38(2)	34(2)	26(2)	-2(1)	-1(1)	9(1)
C(8)	50(2)	40(2)	51(2)	-10(2)	-4(2)	19(2)
C(9)	66(3)	33(2)	58(3)	-17(2)	-2(2)	14(2)
C(10)	55(2)	33(2)	48(2)	-10(2)	-4(2)	-2(2)
C(11)	38(2)	30(1)	29(2)	-3(1)	0(2)	0(1)
C(12)	32(2)	45(2)	40(2)	-6(2)	-4(2)	12(1)
C(13)	46(2)	69(3)	54(3)	2(2)	-11(2)	17(2)
C(14)	45(2)	77(3)	60(3)	13(2)	-12(2)	-11(2)
C(15)	34(2)	38(2)	38(2)	-2(2)	-1(2)	-4(1)
C(16)	47(2)	57(2)	56(3)	5(2)	-1(2)	-14(2)
C(17)	47(2)	48(2)	42(2)	1(2)	-11(2)	1(2)
C(18)	30(2)	19(1)	21(1)	2(1)	0(1)	0(1)
C(19)	32(1)	23(1)	28(2)	1(1)	1(1)	2(1)
C(20)	45(2)	30(2)	33(2)	-7(1)	6(2)	3(1)
C(21)	57(2)	35(2)	34(2)	-9(2)	0(2)	-3(2)
C(22)	41(2)	34(2)	34(2)	-1(1)	-9(2)	-6(1)

C(23)	46(2)	46(2)	51(3)	5(2)	-17(2)	0(2)
C(24)	29(1)	24(1)	26(1)	6(1)	-4(1)	-5(1)
C(25)	32(2)	26(2)	37(2)	-3(1)	4(1)	6(1)
C(27)	36(2)	55(2)	56(3)	-5(2)	16(2)	0(2)
C(28)	29(2)	31(2)	41(2)	4(1)	0(1)	-7(1)
C(29)	40(2)	62(3)	55(3)	15(2)	9(2)	-8(2)
C(30)	33(2)	62(3)	59(3)	20(2)	-5(2)	2(2)
C(31)	25(1)	22(1)	25(1)	7(1)	1(1)	-2(1)
C(32)	28(1)	31(2)	49(2)	1(2)	-10(2)	-2(1)
C(33)	26(1)	40(2)	61(3)	12(2)	-8(2)	-5(1)
C(34)	31(2)	47(2)	47(2)	15(2)	12(2)	8(2)
C(35)	39(2)	54(2)	33(2)	-2(2)	7(2)	15(2)
C(36)	31(2)	40(2)	25(2)	0(1)	-3(1)	4(1)
C(37)	22(1)	26(1)	25(1)	-6(1)	-2(1)	-1(1)
C(38)	30(2)	28(2)	35(2)	-2(1)	-7(1)	-2(1)
C(39)	31(2)	35(2)	45(2)	-9(2)	-2(2)	-7(1)
C(40)	27(2)	50(2)	42(2)	-14(2)	-5(2)	-1(2)
C(41)	35(2)	53(2)	26(2)	-1(2)	-6(1)	3(2)
C(42)	31(2)	34(2)	24(2)	0(1)	-2(1)	1(1)
C(43)	28(1)	21(1)	26(2)	7(1)	-3(1)	-4(1)
C(44)	31(2)	32(2)	38(2)	9(1)	1(1)	-4(1)
C(45)	42(2)	40(2)	54(3)	20(2)	3(2)	-10(2)
C(46)	50(2)	27(2)	60(3)	15(2)	-7(2)	-2(2)
C(47)	45(2)	27(2)	50(2)	6(2)	-9(2)	6(1)
C(48)	32(2)	27(1)	36(2)	5(1)	-3(2)	1(1)
O(2A)	36(2)	63(3)	34(2)	-7(3)	-1(2)	-4(3)
O(3B)	39(3)	38(3)	51(3)	-7(2)	-29(3)	9(2)
O(3A)	37(3)	55(3)	54(4)	32(3)	2(3)	13(2)
F(1)	33(2)	59(4)	40(3)	8(3)	-7(2)	22(2)

Table 54. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Ru(IPr)(PPH_3)$(CO)_2$HF **(45)**.

Atom	x	y	z	U(eq)
H(4)	5213	795	12141	33
H(5)	5292	169	10967	32
H(8)	3171	2250	11551	56
H(9)	4808	2606	12358	63
H(10)	6803	2323	12364	54
H(12)	3429	1276	10117	47
H(13A)	1781	1973	10337	85
H(13B)	1700	1608	9459	85
H(13C)	2800	1947	9405	85
H(14A)	2786	1083	11832	91
H(14B)	1592	1132	11078	91
H(14C)	1931	1494	11919	91
H(15)	7698	1348	11102	44
H(16A)	8426	2028	10558	80
H(16B)	9472	1773	11199	80
H(16C)	8709	2140	11782	80
H(17A)	7931	1655	13247	69
H(17B)	8834	1310	12731	69
H(17C)	7396	1203	12922	69
H(20)	7302	-320	7433	43

H(21)	5372	-513	6739	50
H(22)	3582	-180	7308	44
H(26A)	7820	-129	10268	71
H(26B)	9214	4	9971	71
H(26C)	8519	-352	9289	71
H(25)	7797	513	9345	38
H(27A)	9117	72	7696	73
H(27B)	9597	477	8335	73
H(27C)	8486	521	7490	73
H(28)	3448	681	9176	40
H(29A)	2196	-110	9149	79
H(29B)	1760	295	9810	79
H(29C)	3019	57	10128	79
H(30A)	2882	715	7321	77
H(30B)	1708	737	8106	77
H(30C)	2030	308	7493	77
H(32)	9302	1666	7330	43
H(33)	11240	1404	6837	51
H(34)	11386	897	5503	50
H(35)	9621	683	4580	50
H(36)	7686	962	5020	38
H(38)	5307	822	6473	37
H(39)	3847	553	5286	45
H(40)	3335	921	3743	48
H(41)	4314	1560	3357	45
H(42)	5787	1837	4557	35
H(44)	8475	2074	5278	40
H(45)	8448	2769	4661	54
H(46)	6916	3231	5231	54
H(47)	5365	3003	6407	49
H(48)	5367	2301	7021	38
H(1)	6216	946	8188	53

Table 55. Crystal data and structure refinement for Ru(SIPr)(PPh_3)$(CO)_2$HF **(46)**.

Compound	Ru(SIPr)(PPh_3)$(CO)_2$HF **(46)**
Empirical formula	C57 H54 F N2 O2 P Ru
Formula weight	950.06
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	a = 14.7900(2)Å α = 90°
	b = 17.2450(2)Å β = 103.615(1)°
	c = 18.3490(3)Å γ = 90°
Volume	4548.47(11) $Å^3$
Z	4
Density (calculated)	1.387 Mg/m^3
Absorption coefficient	0.430 mm^{-1}
F(000)	1976
Crystal size	0.25 x 0.25 x 0.05 mm
Theta range for data collection	3.59 to 27.48°
Index ranges	-19<=h<=19; -22<=k<=22; -23<=l<=23
Reflections collected	81674
Independent reflections	10397 [R(int) = 0.0637]
Reflections observed (>2σ)	8014
Data Completeness	0.997
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.98 and 0.89
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10397 / 1 / 519
Goodness-of-fit on F^2	1.038
Final R indices [I>2σ(I)]	R1 = 0.0403 wR2 = 0.0847
R indices (all data)	R1 = 0.0625 wR2 = 0.0935
Largest diff. peak and hole	0.605 and -0.555 $eÅ^{-3}$

Table 56. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIPr)(PPh_3)$(CO)_2$HF **(46)**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	1970(1)	1357(1)	3267(1)	24(1)
P(1)	3164(1)	2285(1)	3527(1)	25(1)
F(1)	2212(1)	1321(1)	2208(1)	37(1)
O(1)	490(1)	2659(1)	2847(2)	61(1)
O(2)	1894(1)	1239(1)	4875(1)	46(1)
N(1)	1577(1)	-392(1)	3114(1)	30(1)
N(2)	284(1)	234(1)	3045(1)	30(1)
C(1)	984(2)	2144(2)	2949(2)	37(1)
C(2)	1897(2)	1309(2)	4250(1)	31(1)
C(3)	1202(2)	324(1)	3091(1)	26(1)
C(4)	908(2)	-1016(2)	3142(2)	41(1)
C(5)	-11(2)	-590(2)	2984(2)	42(1)
C(6)	2523(2)	-581(1)	3086(1)	31(1)
C(7)	3182(2)	-734(2)	3751(2)	36(1)
C(8)	4084(2)	-925(2)	3701(2)	45(1)
C(9)	4317(2)	-976(2)	3019(2)	47(1)

C(10)	3655(2)	-825(2)	2374(2)	45(1)
C(11)	2740(2)	-624(2)	2383(2)	38(1)
C(12)	2963(2)	-700(2)	4517(2)	43(1)
C(13)	3649(2)	-191(2)	5067(2)	58(1)
C(14)	2938(2)	-1526(2)	4827(2)	62(1)
C(15)	2037(2)	-456(2)	1661(2)	51(1)
C(16)	2452(3)	-7(2)	1107(2)	77(1)
C(17)	1575(3)	-1194(3)	1296(2)	81(1)
C(18)	-415(2)	827(2)	2830(1)	32(1)
C(19)	-735(2)	1002(2)	2065(2)	44(1)
C(20)	-1447(2)	1542(2)	1869(2)	51(1)
C(21)	-1832(2)	1892(2)	2399(2)	48(1)
C(22)	-1506(2)	1709(2)	3152(2)	40(1)
C(23)	-785(2)	1182(1)	3382(1)	32(1)
C(24)	-338(2)	628(3)	1461(2)	68(1)
C(25)	-1065(3)	126(3)	940(2)	92(2)
C(26)	83(3)	1223(3)	1026(2)	100(2)
C(27)	-419(2)	1011(2)	4214(1)	34(1)
C(28)	-1059(2)	451(2)	4502(2)	45(1)
C(29)	-269(2)	1752(2)	4688(2)	50(1)
C(30)	4256(2)	1970(1)	3309(1)	28(1)
C(31)	4357(2)	1221(2)	3062(2)	36(1)
C(32)	5173(2)	993(2)	2872(2)	41(1)
C(33)	5888(2)	1509(2)	2921(2)	43(1)
C(34)	5801(2)	2255(2)	3156(2)	53(1)
C(35)	4987(2)	2486(2)	3347(2)	43(1)
C(36)	2960(2)	3201(1)	3009(1)	29(1)
C(37)	3189(2)	3923(2)	3331(2)	42(1)
C(38)	3055(2)	4588(2)	2888(2)	52(1)
C(39)	2710(2)	4533(2)	2128(2)	46(1)
C(40)	2477(2)	3817(2)	1804(2)	44(1)
C(41)	2594(2)	3151(2)	2240(1)	36(1)
C(42)	3453(2)	2574(1)	4510(1)	29(1)
C(43)	2766(2)	2939(2)	4792(2)	41(1)
C(44)	2909(3)	3110(2)	5547(2)	53(1)
C(45)	3740(3)	2917(2)	6031(2)	57(1)
C(46)	4422(3)	2551(2)	5764(2)	55(1)
C(47)	4280(2)	2373(2)	5008(2)	40(1)
C(3S)	4550(4)	5532(4)	4622(4)	120(2)
C(5S)	3545(7)	6498(6)	4972(6)	90(3)
C(1S)	5679(8)	4078(7)	4801(6)	100(3)
C(4S)	3787(9)	6188(8)	4562(8)	119(4)
C(2S)	5309(7)	4943(6)	4629(6)	98(3)

Table 57. Bond lengths [Å] and angles [°] for Ru(SIPr)(PPh_3)$(CO)_2$HF **(46)**.

Ru(1)-H(1)	1.598(9)	C(23)-C(27)	1.524(4)
Ru(1)-C(2)	1.835(3)	C(24)-C(26)	1.522(6)
Ru(1)-C(1)	1.976(3)	C(24)-C(25)	1.528(6)
Ru(1)-F(1)	2.0572(14)	C(27)-C(28)	1.531(4)
Ru(1)-C(3)	2.097(2)	C(27)-C(29)	1.532(4)
Ru(1)-P(1)	2.3480(6)	C(30)-C(31)	1.388(3)
P(1)-C(42)	1.822(2)	C(30)-C(35)	1.389(4)
P(1)-C(36)	1.832(2)	C(31)-C(32)	1.389(4)
P(1)-C(30)	1.835(2)	C(32)-C(33)	1.369(4)

O(1)-C(1)	1.137(3)	C(33)-C(34)	1.372(4)
O(2)-C(2)	1.154(3)	C(34)-C(35)	1.388(4)
N(1)-C(3)	1.350(3)	C(36)-C(37)	1.385(4)
N(1)-C(6)	1.450(3)	C(36)-C(41)	1.390(4)
N(1)-C(4)	1.471(3)	C(37)-C(38)	1.393(4)
N(2)-C(3)	1.349(3)	C(38)-C(39)	1.371(4)
N(2)-C(18)	1.441(3)	C(39)-C(40)	1.378(4)
N(2)-C(5)	1.482(3)	C(40)-C(41)	1.389(4)
C(4)-C(5)	1.512(4)	C(42)-C(47)	1.389(4)
C(6)-C(7)	1.396(4)	C(42)-C(43)	1.393(4)
C(6)-C(11)	1.403(4)	C(43)-C(44)	1.384(4)
C(7)-C(8)	1.397(4)	C(44)-C(45)	1.376(5)
C(7)-C(12)	1.515(4)	C(45)-C(46)	1.375(5)
C(8)-C(9)	1.377(4)	C(46)-C(47)	1.388(4)
C(9)-C(10)	1.373(4)	C(3S)-C(1S)#1	1.362(11)
C(10)-C(11)	1.400(4)	C(3S)-C(2S)	1.512(11)
C(11)-C(15)	1.508(4)	C(3S)-C(2S)#1	1.571(11)
C(12)-C(13)	1.528(4)	C(3S)-C(4S)	1.584(14)
C(12)-C(14)	1.538(4)	C(5S)-C(4S)	1.051(14)
C(15)-C(16)	1.518(5)	C(5S)-C(1S)#1	1.502(14)
C(15)-C(17)	1.522(5)	C(1S)-C(4S)#1	1.329(15)
C(18)-C(23)	1.399(4)	C(1S)-C(3S)#1	1.362(11)
C(18)-C(19)	1.406(4)	C(1S)-C(5S)#1	1.502(14)
C(19)-C(20)	1.388(4)	C(1S)-C(2S)	1.593(15)
C(19)-C(24)	1.515(4)	C(4S)-C(1S)#1	1.329(15)
C(20)-C(21)	1.377(4)	C(2S)-C(3S)#1	1.571(11)
C(21)-C(22)	1.388(4)	C(2S)-C(2S)#1	1.82(2)
C(22)-C(23)	1.390(4)		
H(1)-Ru(1)-C(2)	83.0(9)	C(21)-C(20)-C(19)	121.8(3)
H(1)-Ru(1)-C(1)	173.0(9)	C(20)-C(21)-C(22)	119.9(3)
C(2)-Ru(1)-C(1)	96.39(11)	C(21)-C(22)-C(23)	120.9(3)
H(1)-Ru(1)-F(1)	89.2(9)	C(22)-C(23)-C(18)	118.0(2)
C(2)-Ru(1)-F(1)	172.17(9)	C(22)-C(23)-C(27)	119.8(2)
C(1)-Ru(1)-F(1)	91.34(9)	C(18)-C(23)-C(27)	122.2(2)
H(1)-Ru(1)-C(3)	85.2(9)	C(19)-C(24)-C(26)	111.9(4)
C(2)-Ru(1)-C(3)	87.54(10)	C(19)-C(24)-C(25)	111.2(3)
C(1)-Ru(1)-C(3)	101.71(10)	C(26)-C(24)-C(25)	111.6(3)
F(1)-Ru(1)-C(3)	92.16(7)	C(23)-C(27)-C(28)	111.4(2)
H(1)-Ru(1)-P(1)	79.7(9)	C(23)-C(27)-C(29)	112.2(2)
C(2)-Ru(1)-P(1)	92.67(8)	C(28)-C(27)-C(29)	110.4(2)
C(1)-Ru(1)-P(1)	93.44(8)	C(31)-C(30)-C(35)	118.0(2)
F(1)-Ru(1)-P(1)	85.56(4)	C(31)-C(30)-P(1)	121.00(19)
C(3)-Ru(1)-P(1)	164.74(7)	C(35)-C(30)-P(1)	120.9(2)
C(42)-P(1)-C(36)	104.41(11)	C(30)-C(31)-C(32)	120.8(2)
C(42)-P(1)-C(30)	106.49(11)	C(33)-C(32)-C(31)	120.2(3)
C(36)-P(1)-C(30)	100.89(11)	C(32)-C(33)-C(34)	120.1(3)
C(42)-P(1)-Ru(1)	112.17(8)	C(33)-C(34)-C(35)	120.0(3)
C(36)-P(1)-Ru(1)	117.25(8)	C(30)-C(35)-C(34)	121.0(3)
C(30)-P(1)-Ru(1)	114.35(8)	C(37)-C(36)-C(41)	119.2(2)
C(3)-N(1)-C(6)	126.7(2)	C(37)-C(36)-P(1)	124.05(19)
C(3)-N(1)-C(4)	113.3(2)	C(41)-C(36)-P(1)	116.71(19)
C(6)-N(1)-C(4)	120.0(2)	C(36)-C(37)-C(38)	120.3(3)
C(3)-N(2)-C(18)	125.6(2)	C(39)-C(38)-C(37)	120.3(3)
C(3)-N(2)-C(5)	112.9(2)	C(38)-C(39)-C(40)	119.8(3)
C(18)-N(2)-C(5)	118.6(2)	C(39)-C(40)-C(41)	120.5(3)

O(1)-C(1)-Ru(1)	170.3(3)	C(40)-C(41)-C(36)	119.9(3)
O(2)-C(2)-Ru(1)	175.5(2)	C(47)-C(42)-C(43)	118.4(2)
N(2)-C(3)-N(1)	107.3(2)	C(47)-C(42)-P(1)	123.2(2)
N(2)-C(3)-Ru(1)	127.43(18)	C(43)-C(42)-P(1)	118.0(2)
N(1)-C(3)-Ru(1)	124.67(17)	C(44)-C(43)-C(42)	121.0(3)
N(1)-C(4)-C(5)	102.6(2)	C(45)-C(44)-C(43)	119.9(3)
N(2)-C(5)-C(4)	102.5(2)	C(44)-C(45)-C(46)	120.0(3)
C(7)-C(6)-C(11)	122.0(2)	C(45)-C(46)-C(47)	120.5(3)
C(7)-C(6)-N(1)	119.5(2)	C(42)-C(47)-C(46)	120.4(3)
C(11)-C(6)-N(1)	118.4(2)	C(1S)#1-C(3S)-C(2S)	130.1(8)
C(6)-C(7)-C(8)	117.9(2)	C(1S)#1-C(3S)-C(2S)#1	65.4(7)
C(6)-C(7)-C(12)	123.1(2)	C(2S)-C(3S)-C(2S)#1	72.4(7)
C(8)-C(7)-C(12)	119.1(2)	C(1S)#1-C(3S)-C(4S)	53.0(7)
C(9)-C(8)-C(7)	121.4(3)	C(2S)-C(3S)-C(4S)	175.1(8)
C(10)-C(9)-C(8)	119.5(3)	C(2S)#1-C(3S)-C(4S)	112.3(8)
C(9)-C(10)-C(11)	122.1(3)	C(4S)-C(5S)-C(1S)#1	59.7(10)
C(10)-C(11)-C(6)	117.1(3)	C(4S)#1-C(1S)-C(3S)#1	72.1(9)
C(10)-C(11)-C(15)	120.4(3)	C(4S)#1-C(1S)-C(5S)#1	43.1(7)
C(6)-C(11)-C(15)	122.6(3)	C(3S)#1-C(1S)-C(5S)#1	115.1(9)
C(7)-C(12)-C(13)	112.4(2)	C(4S)#1-C(1S)-C(2S)	127.1(11)
C(7)-C(12)-C(14)	109.6(3)	C(3S)#1-C(1S)-C(2S)	63.6(6)
C(13)-C(12)-C(14)	111.0(3)	C(5S)#1-C(1S)-C(2S)	151.5(10)
C(11)-C(15)-C(16)	112.5(3)	C(5S)-C(4S)-C(1S)#1	77.2(11)
C(11)-C(15)-C(17)	111.8(3)	C(5S)-C(4S)-C(3S)	132.1(13)
C(16)-C(15)-C(17)	110.0(3)	C(1S)#1-C(4S)-C(3S)	54.9(7)
C(23)-C(18)-C(19)	122.1(3)	C(3S)-C(2S)-C(3S)#1	107.6(7)
C(23)-C(18)-N(2)	119.4(2)	C(3S)-C(2S)-C(1S)	148.2(9)
C(19)-C(18)-N(2)	118.4(2)	C(3S)#1-C(2S)-C(1S)	51.0(6)
C(20)-C(19)-C(18)	117.4(3)	C(3S)-C(2S)-C(2S)#1	55.3(6)
C(20)-C(19)-C(24)	119.8(3)	C(3S)#1-C(2S)-C(2S)#1	52.3(6)
C(18)-C(19)-C(24)	122.8(3)	C(1S)-C(2S)-C(2S)#1	99.4(9)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

Table 58. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(SIPr)(PPh_3)(CO)_2HF$ **(46)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	23(1)	24(1)	25(1)	2(1)	4(1)	-1(1)
P(1)	25(1)	23(1)	26(1)	2(1)	5(1)	0(1)
F(1)	44(1)	39(1)	28(1)	0(1)	9(1)	-7(1)
O(1)	37(1)	40(1)	104(2)	22(1)	13(1)	10(1)
O(2)	50(1)	59(1)	30(1)	0(1)	10(1)	-17(1)
N(1)	32(1)	24(1)	33(1)	2(1)	5(1)	-4(1)
N(2)	27(1)	30(1)	31(1)	-2(1)	6(1)	-6(1)
C(1)	28(1)	36(2)	43(2)	11(1)	4(1)	-6(1)
C(2)	28(1)	31(1)	31(1)	0(1)	3(1)	-7(1)
C(3)	28(1)	30(1)	19(1)	1(1)	3(1)	-3(1)
C(4)	41(2)	29(1)	54(2)	-2(1)	14(1)	-9(1)
C(5)	38(2)	34(1)	53(2)	-4(1)	11(1)	-13(1)
C(6)	36(1)	20(1)	39(1)	0(1)	11(1)	0(1)
C(7)	36(1)	33(1)	40(2)	3(1)	12(1)	4(1)
C(8)	38(2)	49(2)	49(2)	3(1)	10(1)	8(1)

C(9)	48(2)	41(2)	59(2)	2(1)	26(2)	11(1)
C(10)	67(2)	29(1)	47(2)	1(1)	33(2)	9(1)
C(11)	56(2)	23(1)	37(2)	1(1)	14(1)	4(1)
C(12)	33(1)	62(2)	34(2)	10(1)	7(1)	11(1)
C(13)	41(2)	96(3)	36(2)	-1(2)	4(1)	11(2)
C(14)	54(2)	77(2)	59(2)	34(2)	22(2)	23(2)
C(15)	73(2)	46(2)	33(2)	-2(1)	11(1)	19(2)
C(16)	139(4)	48(2)	39(2)	7(2)	10(2)	-14(2)
C(17)	86(3)	89(3)	55(2)	12(2)	-7(2)	-31(2)
C(18)	23(1)	39(1)	33(1)	2(1)	4(1)	-8(1)
C(19)	30(1)	69(2)	32(1)	3(1)	2(1)	-1(1)
C(20)	30(2)	79(2)	41(2)	17(2)	1(1)	1(2)
C(21)	29(1)	51(2)	60(2)	16(2)	4(1)	1(1)
C(22)	30(1)	41(2)	51(2)	4(1)	12(1)	-1(1)
C(23)	26(1)	32(1)	37(1)	3(1)	7(1)	-7(1)
C(24)	45(2)	127(3)	29(2)	1(2)	2(1)	21(2)
C(25)	82(3)	132(4)	52(2)	-29(3)	-1(2)	26(3)
C(26)	64(3)	195(6)	43(2)	7(3)	19(2)	-6(3)
C(27)	32(1)	38(1)	33(1)	-1(1)	9(1)	-3(1)
C(28)	43(2)	53(2)	40(2)	5(1)	14(1)	-6(1)
C(29)	56(2)	48(2)	45(2)	-9(1)	10(1)	-3(2)
C(30)	26(1)	29(1)	28(1)	6(1)	6(1)	1(1)
C(31)	32(1)	30(1)	46(2)	-3(1)	13(1)	-2(1)
C(32)	36(2)	37(2)	55(2)	-2(1)	17(1)	2(1)
C(33)	31(1)	45(2)	57(2)	11(1)	19(1)	7(1)
C(34)	33(2)	38(2)	91(3)	10(2)	24(2)	-4(1)
C(35)	33(2)	28(1)	70(2)	3(1)	17(1)	0(1)
C(36)	26(1)	27(1)	33(1)	4(1)	8(1)	1(1)
C(37)	52(2)	29(1)	40(2)	4(1)	-2(1)	-2(1)
C(38)	66(2)	26(1)	56(2)	6(1)	-2(2)	-5(1)
C(39)	47(2)	34(2)	54(2)	18(1)	6(1)	2(1)
C(40)	54(2)	42(2)	36(2)	12(1)	7(1)	4(1)
C(41)	41(2)	34(1)	33(1)	4(1)	9(1)	2(1)
C(42)	35(1)	23(1)	30(1)	0(1)	8(1)	-6(1)
C(43)	42(2)	39(2)	46(2)	-12(1)	14(1)	-5(1)
C(44)	72(2)	40(2)	56(2)	-20(2)	33(2)	-16(2)
C(45)	97(3)	43(2)	32(2)	-7(1)	16(2)	-18(2)
C(46)	77(2)	46(2)	34(2)	2(1)	-6(2)	-1(2)
C(47)	48(2)	36(1)	31(1)	1(1)	2(1)	0(1)

Table 59. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIPr)(PPh_3)$(CO)_2$HF **(46)**.

Atom	x	y	z	U(eq)
H(4A)	1041	-1266	3641	49
H(4B)	916	-1415	2755	49
H(5A)	-390	-710	2476	50
H(5B)	-371	-720	3359	50
H(8)	4546	-1022	4148	54
H(9)	4931	-1114	2996	56
H(10)	3822	-858	1905	54
H(12)	2329	-469	4454	51
H(13A)	4263	-437	5184	88
H(13B)	3432	-128	5528	88

H(13C)	3690	319	4840	88
H(14A)	2472	-1833	4476	93
H(14B)	2774	-1504	5314	93
H(14C)	3551	-1767	4887	93
H(15)	1539	-126	1787	61
H(16A)	2834	419	1368	115
H(16B)	1950	205	710	115
H(16C)	2838	-354	885	115
H(17A)	2048	-1537	1177	121
H(17B)	1116	-1062	834	121
H(17C)	1264	-1458	1643	121
H(20)	-1673	1674	1356	61
H(21)	-2321	2258	2249	57
H(22)	-1778	1948	3514	49
H(24)	176	276	1717	81
H(25A)	-1317	-254	1237	137
H(25B)	-775	-146	584	137
H(25C)	-1570	456	663	137
H(26A)	-386	1614	813	150
H(26B)	294	964	620	150
H(26C)	614	1476	1364	150
H(27)	200	752	4277	41
H(28A)	-1688	668	4404	67
H(28B)	-823	373	5042	67
H(28C)	-1075	-48	4243	67
H(29A)	107	2119	4477	75
H(29B)	54	1625	5204	75
H(29C)	-873	1987	4686	75
H(31)	3863	860	3023	43
H(32)	5235	478	2708	49
H(33)	6445	1351	2791	51
H(34)	6297	2613	3189	63
H(35)	4929	3004	3505	51
H(37)	3439	3964	3856	51
H(38)	3202	5082	3114	62
H(39)	2632	4987	1826	55
H(40)	2234	3780	1278	53
H(41)	2425	2660	2013	43
H(43)	2191	3073	4460	50
H(44)	2435	3359	5732	64
H(45)	3841	3037	6550	69
H(46)	4995	2419	6100	66
H(47)	4752	2111	4831	47
H(1)	2851(11)	808(12)	3556(13)	27(6)

Table 60. Crystal data and structure refinement for $Ru(IPr)(PPh_3)_2(CO)H_2$ **(47)**.

Compound	$Ru(IPr)(PPh_3)_2(CO)H_2$ **(47)**
Empirical formula	C68 H76 N2 O2 P2 Ru
Formula weight	1116.32
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P21cn
Unit cell dimensions	a = 11.6010(1)Å α = 90°
	b = 12.6060(2)Å β = 90°
	c = 39.3500(6)Å γ = 90°
Volume	5754.63(14) $Å^3$
Z	4
Density (calculated)	1.288 Mg/m^3
Absorption coefficient	0.375 mm^{-1}
F(000)	2352
Crystal size	0.15 x 0.07 x 0.07 mm
Theta range for data collection	3.52 to 25.00 °.
Index ranges	-13<=h<=13; -14<=k<=14; -45<=l<=46
Reflections collected	60542
Independent reflections	10099 [R(int) = 0.0914]
Reflections observed (>2σ)	7990
Data Completeness	0.996
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.96 and 0.93
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10099 / 15 / 689
Goodness-of-fit on F^2	1.062
Final R indices [I>2σ(I)]	R^1 = 0.0470 wR_2 = 0.0792
R indices (all data)	R^1 = 0.0730 wR_2 = 0.0874
Absolute structure parameter	-0.03(3)
Largest diff. peak and hole	0.528 and -0.461 $eÅ^{-3}$

Table 61. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IPr)(PPh_3)_2(CO)H_2$ **(47)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	5255(1)	2389(1)	3768(1)	21(1)
P(1)	5702(1)	1679(1)	3222(1)	23(1)
P(2)	4943(1)	4156(1)	3617(1)	23(1)
O(1)	7709(3)	2935(3)	3995(1)	38(1)
O(2)	585(4)	4831(4)	4590(1)	75(1)
N(1)	3885(3)	610(3)	4137(1)	23(1)
N(2)	5673(3)	448(3)	4277(1)	24(1)
C(1)	6777(4)	2683(4)	3917(1)	28(1)
C(2)	4963(4)	1053(3)	4069(1)	23(1)
C(3)	3950(4)	-222(4)	4365(1)	29(1)
C(4)	5070(4)	-329(3)	4448(1)	31(1)
C(5)	2759(4)	1081(3)	4063(1)	26(1)
C(6)	2366(4)	1854(4)	4286(1)	27(1)
C(7)	1293(4)	2310(4)	4221(1)	37(1)
C(8)	637(4)	1985(4)	3946(1)	39(1)

C(9)	1028(4)	1189(4)	3735(1)	35(1)
C(10)	2105(4)	709(4)	3790(1)	31(1)
C(11)	2989(4)	2132(4)	4613(1)	36(1)
C(12)	2432(5)	1584(5)	4913(1)	48(2)
C(13)	3063(5)	3336(4)	4678(1)	49(2)
C(14)	2505(4)	-215(4)	3571(1)	38(1)
C(15)	1980(6)	-1256(5)	3700(1)	61(2)
C(16)	2243(5)	-66(5)	3194(1)	51(2)
C(17)	6893(4)	598(4)	4363(1)	27(1)
C(18)	7160(4)	1352(4)	4609(1)	31(1)
C(19)	8320(5)	1423(4)	4711(1)	41(1)
C(20)	9146(5)	757(5)	4578(1)	45(1)
C(21)	8841(4)	17(4)	4338(1)	39(1)
C(22)	7708(4)	-91(4)	4227(1)	33(1)
C(23)	6276(4)	2072(4)	4775(1)	37(1)
C(24)	5728(5)	1507(4)	5079(1)	48(1)
C(25)	6758(5)	3152(4)	4891(1)	51(2)
C(26)	7430(4)	-976(4)	3974(1)	38(1)
C(27)	7669(6)	-2075(4)	4116(1)	58(2)
C(28)	8108(5)	-809(6)	3642(1)	66(2)
C(29)	5335(5)	282(3)	3112(1)	27(1)
C(30)	5383(5)	-483(3)	3368(1)	32(1)
C(31)	5257(5)	-1547(3)	3295(1)	41(1)
C(32)	5037(5)	-1859(4)	2965(1)	46(2)
C(33)	4966(5)	-1114(4)	2713(1)	48(2)
C(34)	5125(5)	-60(3)	2785(1)	38(1)
C(35)	7226(4)	1708(4)	3082(1)	24(1)
C(36)	7770(4)	908(4)	2903(1)	34(1)
C(37)	8923(4)	978(4)	2813(1)	40(1)
C(38)	9567(4)	1860(4)	2904(1)	37(1)
C(39)	9033(4)	2679(4)	3082(1)	34(1)
C(40)	7882(4)	2599(4)	3169(1)	28(1)
C(41)	4975(4)	2317(3)	2857(1)	26(1)
C(42)	5530(4)	2537(3)	2548(1)	33(1)
C(43)	4937(5)	2967(4)	2277(1)	42(2)
C(44)	3773(5)	3183(4)	2307(1)	43(1)
C(45)	3206(5)	2969(4)	2612(1)	36(1)
C(46)	3809(4)	2547(3)	2883(1)	28(1)
C(47)	4929(4)	5114(3)	3978(1)	25(1)
C(48)	5459(5)	4882(4)	4280(1)	39(1)
C(49)	5489(5)	5605(4)	4547(1)	49(2)
C(50)	4970(5)	6562(4)	4514(1)	47(2)
C(51)	4428(5)	6821(5)	4214(2)	66(2)
C(52)	4419(5)	6098(4)	3947(1)	51(2)
C(53)	3543(4)	4519(3)	3424(1)	24(1)
C(54)	2565(4)	3980(4)	3536(1)	28(1)
C(55)	1480(4)	4272(4)	3423(1)	37(1)
C(56)	1335(4)	5081(4)	3192(1)	42(1)
C(57)	2301(5)	5616(4)	3075(1)	42(1)
C(58)	3381(4)	5348(4)	3195(1)	36(1)
C(59)	6007(4)	4837(3)	3342(1)	26(1)
C(60)	6966(4)	5308(4)	3482(1)	32(1)
C(61)	7842(4)	5695(4)	3282(1)	37(1)
C(62)	7772(5)	5632(4)	2934(1)	44(1)
C(63)	6812(5)	5174(4)	2786(1)	38(1)

C(64)	5949(4)	4772(3)	2987(1)	29(1)
C(65)	950(20)	5374(17)	4299(4)	72(7)
C(66)	-172(18)	5800(30)	4153(9)	211(16)
C(67)	-1197(15)	5358(13)	4351(4)	65(5)
C(68)	-684(10)	4581(11)	4609(4)	48(4)
C(65A)	1345(11)	5302(10)	4321(3)	64(5)
C(66A)	508(10)	6051(9)	4134(3)	91(4)
C(67A)	-554(10)	5322(9)	4130(3)	72(4)
C(68A)	-580(9)	4783(11)	4471(3)	79(4)

Table 62. Bond lengths [Å] and angles [°] for Ru(IPr)(PPh_3)$_2$(CO)H_2 **(47)**.

Ru(1)-H(2)	1.592(10)	C(23)-C(25)	1.542(7)
Ru(1)-H(1)	1.602(10)	C(26)-C(27)	1.520(7)
Ru(1)-C(1)	1.897(5)	C(26)-C(28)	1.540(7)
Ru(1)-C(2)	2.087(4)	C(29)-C(34)	1.381(5)
Ru(1)-P(2)	2.3333(12)	C(29)-C(30)	1.394(5)
Ru(1)-P(1)	2.3832(11)	C(30)-C(31)	1.380(6)
P(1)-C(41)	1.850(4)	C(31)-C(32)	1.382(6)
P(1)-C(35)	1.853(4)	C(32)-C(33)	1.369(6)
P(1)-C(29)	1.862(4)	C(33)-C(34)	1.371(6)
P(2)-C(53)	1.850(4)	C(35)-C(36)	1.384(6)
P(2)-C(59)	1.851(5)	C(35)-C(40)	1.399(6)
P(2)-C(47)	1.866(4)	C(36)-C(37)	1.385(6)
O(1)-C(1)	1.169(5)	C(37)-C(38)	1.386(7)
O(2)-C(65)	1.401(13)	C(38)-C(39)	1.394(6)
O(2)-C(68A)	1.432(10)	C(39)-C(40)	1.382(6)
O(2)-C(65A)	1.500(10)	C(41)-C(46)	1.387(6)
O(2)-C(68)	1.507(11)	C(41)-C(42)	1.402(6)
N(1)-C(3)	1.383(5)	C(42)-C(43)	1.382(6)
N(1)-C(2)	1.395(5)	C(43)-C(44)	1.383(7)
N(1)-C(5)	1.464(6)	C(44)-C(45)	1.397(7)
N(2)-C(4)	1.379(5)	C(45)-C(46)	1.383(6)
N(2)-C(2)	1.389(5)	C(47)-C(48)	1.370(6)
N(2)-C(17)	1.467(5)	C(47)-C(52)	1.380(6)
C(3)-C(4)	1.347(7)	C(48)-C(49)	1.389(6)
C(5)-C(6)	1.388(6)	C(49)-C(50)	1.355(7)
C(5)-C(10)	1.397(6)	C(50)-C(51)	1.374(7)
C(6)-C(7)	1.395(6)	C(51)-C(52)	1.391(7)
C(6)-C(11)	1.515(6)	C(53)-C(58)	1.392(6)
C(7)-C(8)	1.385(7)	C(53)-C(54)	1.394(6)
C(8)-C(9)	1.379(6)	C(54)-C(55)	1.386(6)
C(9)-C(10)	1.405(6)	C(55)-C(56)	1.376(7)
C(10)-C(14)	1.523(7)	C(56)-C(57)	1.387(7)
C(11)-C(12)	1.514(6)	C(57)-C(58)	1.381(7)
C(11)-C(13)	1.541(7)	C(59)-C(60)	1.376(6)
C(14)-C(16)	1.524(6)	C(59)-C(64)	1.401(6)
C(14)-C(15)	1.534(7)	C(60)-C(61)	1.376(6)
C(17)-C(22)	1.390(6)	C(61)-C(62)	1.373(7)
C(17)-C(18)	1.393(6)	C(62)-C(63)	1.382(7)
C(18)-C(19)	1.408(6)	C(63)-C(64)	1.373(6)
C(18)-C(23)	1.517(7)	C(65)-C(66)	1.522(10)
C(19)-C(20)	1.378(7)	C(66)-C(67)	1.528(10)
C(20)-C(21)	1.373(7)	C(67)-C(68)	1.532(9)
C(21)-C(22)	1.392(7)	C(65A)-C(66A)	1.542(9)

C(22)-C(26)	1.530(7)	C(66A)-C(67A)	1.537(9)
C(23)-C(24)	1.532(7)	C(67A)-C(68A)	1.503(9)
H(2)-Ru(1)-H(1)	88(2)	C(20)-C(19)-C(18)	121.1(5)
H(2)-Ru(1)-C(1)	96.0(16)	C(21)-C(20)-C(19)	119.8(5)
H(1)-Ru(1)-C(1)	175.1(16)	C(20)-C(21)-C(22)	121.7(5)
H(2)-Ru(1)-C(2)	78.3(15)	C(17)-C(22)-C(21)	117.4(5)
H(1)-Ru(1)-C(2)	85.3(16)	C(17)-C(22)-C(26)	124.2(4)
C(1)-Ru(1)-C(2)	97.63(17)	C(21)-C(22)-C(26)	118.3(5)
H(2)-Ru(1)-P(2)	75.5(15)	C(18)-C(23)-C(24)	109.8(4)
H(1)-Ru(1)-P(2)	86.9(16)	C(18)-C(23)-C(25)	114.3(4)
C(1)-Ru(1)-P(2)	92.13(14)	C(24)-C(23)-C(25)	109.1(4)
C(2)-Ru(1)-P(2)	152.83(11)	C(27)-C(26)-C(22)	112.8(4)
H(2)-Ru(1)-P(1)	164.6(15)	C(27)-C(26)-C(28)	110.1(5)
H(1)-Ru(1)-P(1)	76.8(16)	C(22)-C(26)-C(28)	110.2(5)
C(1)-Ru(1)-P(1)	98.65(14)	C(34)-C(29)-C(30)	117.6(4)
C(2)-Ru(1)-P(1)	104.11(11)	C(34)-C(29)-P(1)	123.5(3)
P(2)-Ru(1)-P(1)	99.36(4)	C(30)-C(29)-P(1)	118.5(3)
C(41)-P(1)-C(35)	101.23(19)	C(31)-C(30)-C(29)	121.2(4)
C(41)-P(1)-C(29)	97.27(18)	C(30)-C(31)-C(32)	119.5(4)
C(35)-P(1)-C(29)	99.7(2)	C(33)-C(32)-C(31)	119.8(4)
C(41)-P(1)-Ru(1)	115.94(13)	C(32)-C(33)-C(34)	120.5(4)
C(35)-P(1)-Ru(1)	117.91(14)	C(33)-C(34)-C(29)	121.3(4)
C(29)-P(1)-Ru(1)	120.98(13)	C(36)-C(35)-C(40)	117.5(4)
C(53)-P(2)-C(59)	103.4(2)	C(36)-C(35)-P(1)	125.0(4)
C(53)-P(2)-C(47)	98.31(19)	C(40)-C(35)-P(1)	117.6(3)
C(59)-P(2)-C(47)	98.6(2)	C(35)-C(36)-C(37)	121.6(5)
C(53)-P(2)-Ru(1)	118.47(15)	C(36)-C(37)-C(38)	120.4(5)
C(59)-P(2)-Ru(1)	119.23(15)	C(37)-C(38)-C(39)	118.9(5)
C(47)-P(2)-Ru(1)	115.15(14)	C(40)-C(39)-C(38)	120.0(5)
C(65)-O(2)-C(68A)	92.1(11)	C(39)-C(40)-C(35)	121.6(4)
C(65)-O(2)-C(65A)	18.5(11)	C(46)-C(41)-C(42)	118.2(4)
C(68A)-O(2)-C(65A)	109.9(8)	C(46)-C(41)-P(1)	118.5(3)
C(65)-O(2)-C(68)	116.0(12)	C(42)-C(41)-P(1)	123.3(3)
C(68A)-O(2)-C(68)	23.9(6)	C(43)-C(42)-C(41)	121.2(4)
C(65A)-O(2)-C(68)	133.8(8)	C(42)-C(43)-C(44)	119.8(5)
C(3)-N(1)-C(2)	112.3(4)	C(43)-C(44)-C(45)	119.7(5)
C(3)-N(1)-C(5)	119.0(4)	C(46)-C(45)-C(44)	120.0(5)
C(2)-N(1)-C(5)	126.8(3)	C(45)-C(46)-C(41)	121.1(5)
C(4)-N(2)-C(2)	112.1(4)	C(48)-C(47)-C(52)	117.3(4)
C(4)-N(2)-C(17)	117.9(4)	C(48)-C(47)-P(2)	121.3(3)
C(2)-N(2)-C(17)	129.5(4)	C(52)-C(47)-P(2)	121.3(3)
O(1)-C(1)-Ru(1)	174.8(4)	C(47)-C(48)-C(49)	121.8(4)
N(2)-C(2)-N(1)	101.5(3)	C(50)-C(49)-C(48)	120.1(5)
N(2)-C(2)-Ru(1)	132.9(3)	C(49)-C(50)-C(51)	119.7(5)
N(1)-C(2)-Ru(1)	125.3(3)	C(50)-C(51)-C(52)	119.7(5)
C(4)-C(3)-N(1)	106.6(4)	C(47)-C(52)-C(51)	121.4(5)
C(3)-C(4)-N(2)	107.5(4)	C(58)-C(53)-C(54)	117.5(4)
C(6)-C(5)-C(10)	122.9(4)	C(58)-C(53)-P(2)	124.7(4)
C(6)-C(5)-N(1)	116.9(4)	C(54)-C(53)-P(2)	117.6(3)
C(10)-C(5)-N(1)	120.1(4)	C(55)-C(54)-C(53)	120.5(4)
C(5)-C(6)-C(7)	117.7(4)	C(56)-C(55)-C(54)	121.4(5)
C(5)-C(6)-C(11)	122.8(4)	C(55)-C(56)-C(57)	118.7(5)
C(7)-C(6)-C(11)	119.2(4)	C(58)-C(57)-C(56)	120.1(5)
C(8)-C(7)-C(6)	120.9(5)	C(57)-C(58)-C(53)	121.8(5)

C(9)-C(8)-C(7)	120.3(5)	C(60)-C(59)-C(64)	117.6(4)
C(8)-C(9)-C(10)	120.8(4)	C(60)-C(59)-P(2)	120.3(3)
C(5)-C(10)-C(9)	117.3(4)	C(64)-C(59)-P(2)	121.5(3)
C(5)-C(10)-C(14)	121.8(4)	C(61)-C(60)-C(59)	121.4(4)
C(9)-C(10)-C(14)	120.8(4)	C(62)-C(61)-C(60)	120.4(5)
C(12)-C(11)-C(6)	110.7(4)	C(61)-C(62)-C(63)	119.5(5)
C(12)-C(11)-C(13)	110.0(4)	C(64)-C(63)-C(62)	119.9(5)
C(6)-C(11)-C(13)	113.4(4)	C(63)-C(64)-C(59)	121.2(5)
C(10)-C(14)-C(16)	113.3(4)	O(2)-C(65)-C(66)	102.9(17)
C(10)-C(14)-C(15)	110.2(4)	C(65)-C(66)-C(67)	110.1(19)
C(16)-C(14)-C(15)	110.4(4)	C(66)-C(67)-C(68)	105.6(16)
C(22)-C(17)-C(18)	122.9(4)	O(2)-C(68)-C(67)	102.3(10)
C(22)-C(17)-N(2)	119.1(4)	O(2)-C(65A)-C(66A)	102.0(9)
C(18)-C(17)-N(2)	117.5(4)	C(67A)-C(66A)-C(65A)	98.3(9)
C(17)-C(18)-C(19)	117.1(5)	C(68A)-C(67A)-C(66A)	106.0(9)
C(17)-C(18)-C(23)	123.9(4)	O(2)-C(68A)-C(67A)	104.8(9)
C(19)-C(18)-C(23)	119.0(4)		

Table 63. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IPr)(PPh_3)_2(CO)H_2$ **(47)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	21(1)	22(1)	19(1)	0(1)	0(1)	0(1)
P(1)	25(1)	23(1)	22(1)	-1(1)	0(1)	0(1)
P(2)	25(1)	24(1)	22(1)	0(1)	1(1)	-1(1)
O(1)	28(2)	47(2)	38(2)	3(2)	-7(2)	-9(2)
O(2)	58(3)	99(3)	67(3)	-15(2)	0(2)	-8(3)
N(1)	23(2)	24(2)	20(2)	4(2)	1(2)	-1(2)
N(2)	25(2)	22(2)	26(2)	2(2)	-1(2)	1(2)
C(1)	34(3)	25(3)	24(2)	5(2)	3(2)	0(2)
C(2)	20(3)	26(2)	21(2)	-3(2)	-3(2)	3(2)
C(3)	28(3)	27(3)	32(3)	7(2)	4(2)	-8(2)
C(4)	32(3)	31(2)	30(2)	6(2)	1(2)	1(3)
C(5)	24(3)	28(3)	27(3)	10(2)	0(2)	-5(2)
C(6)	21(3)	30(3)	30(3)	8(2)	5(2)	-2(2)
C(7)	37(3)	35(3)	39(3)	3(2)	10(2)	0(3)
C(8)	28(3)	48(3)	40(3)	11(2)	4(2)	2(2)
C(9)	29(3)	48(3)	27(3)	10(2)	-9(2)	-6(2)
C(10)	21(2)	41(3)	31(3)	11(2)	6(2)	-3(2)
C(11)	29(3)	49(3)	31(3)	-3(2)	3(2)	-1(2)
C(12)	43(4)	70(4)	32(3)	4(3)	1(3)	-2(3)
C(13)	41(4)	57(4)	51(4)	-17(3)	12(3)	-4(3)
C(14)	26(3)	45(3)	44(3)	-8(3)	-5(2)	-1(2)
C(15)	88(5)	45(4)	51(4)	-5(3)	-9(3)	13(3)
C(16)	52(4)	66(4)	35(3)	-20(3)	3(3)	-19(3)
C(17)	19(2)	32(3)	29(3)	11(2)	-3(2)	0(2)
C(18)	30(3)	27(3)	35(3)	8(2)	-9(2)	-3(2)
C(19)	38(3)	34(3)	51(3)	12(3)	-14(3)	-4(3)
C(20)	30(3)	55(4)	49(3)	21(3)	-11(3)	-10(3)
C(21)	23(3)	56(4)	38(3)	17(3)	2(2)	4(3)
C(22)	32(3)	39(3)	29(3)	13(2)	1(2)	3(3)
C(23)	41(3)	35(3)	34(3)	0(2)	-10(2)	-3(3)
C(24)	49(3)	52(4)	43(3)	0(3)	-1(3)	5(3)

C(25)	58(4)	44(4)	51(3)	-8(3)	-13(3)	-4(3)
C(26)	29(3)	55(4)	31(3)	-2(2)	-4(2)	18(3)
C(27)	71(4)	44(4)	60(4)	-14(3)	-17(3)	19(3)
C(28)	57(4)	113(6)	27(3)	0(4)	9(3)	12(4)
C(29)	23(3)	29(2)	28(2)	-1(2)	4(2)	-2(3)
C(30)	37(3)	30(2)	29(2)	0(2)	0(3)	0(3)
C(31)	60(3)	25(2)	39(3)	7(2)	10(3)	5(4)
C(32)	64(4)	23(2)	50(3)	-8(2)	5(3)	-14(3)
C(33)	76(5)	37(3)	30(3)	-5(2)	-8(3)	-13(3)
C(34)	55(4)	34(3)	27(2)	-1(2)	-5(3)	-6(3)
C(35)	25(3)	26(3)	22(2)	2(2)	1(2)	0(2)
C(36)	35(3)	28(3)	39(3)	0(2)	11(2)	-1(2)
C(37)	40(3)	33(3)	46(3)	1(2)	14(3)	13(3)
C(38)	27(3)	45(3)	38(3)	17(2)	4(2)	3(2)
C(39)	32(3)	40(3)	30(3)	6(2)	-2(2)	-9(2)
C(40)	32(3)	28(3)	25(2)	0(2)	3(2)	-4(2)
C(41)	35(3)	18(2)	25(2)	-5(2)	-2(2)	-2(2)
C(42)	43(4)	28(2)	28(2)	-6(2)	-1(2)	0(2)
C(43)	68(5)	33(3)	25(3)	4(2)	-3(3)	-6(3)
C(44)	66(4)	26(3)	38(3)	-1(2)	-24(3)	2(3)
C(45)	44(3)	27(3)	37(3)	-4(2)	-14(3)	6(2)
C(46)	38(3)	24(3)	24(2)	0(2)	-7(2)	2(2)
C(47)	23(3)	24(2)	27(2)	2(2)	3(2)	-4(2)
C(48)	61(4)	24(2)	31(3)	-4(2)	-1(3)	9(3)
C(49)	76(5)	42(3)	27(2)	-5(2)	-8(3)	1(3)
C(50)	55(4)	36(3)	50(3)	-20(2)	7(3)	-3(3)
C(51)	73(5)	48(4)	76(4)	-30(3)	-34(4)	28(3)
C(52)	69(4)	33(3)	52(3)	-15(3)	-28(3)	11(3)
C(53)	29(3)	23(3)	21(2)	0(2)	-1(2)	3(2)
C(54)	27(3)	30(3)	27(3)	1(2)	-2(2)	1(2)
C(55)	22(3)	43(3)	44(3)	0(3)	-3(2)	3(2)
C(56)	23(3)	57(4)	45(3)	-1(3)	-6(3)	10(3)
C(57)	39(3)	53(4)	35(3)	8(3)	-9(3)	21(3)
C(58)	32(3)	38(3)	37(3)	8(2)	-1(2)	2(2)
C(59)	27(3)	17(2)	33(3)	-4(2)	1(2)	0(2)
C(60)	35(3)	29(3)	32(3)	1(2)	4(2)	-5(2)
C(61)	29(3)	34(3)	48(3)	3(3)	7(2)	-6(2)
C(62)	40(3)	35(3)	58(4)	4(3)	15(3)	-3(3)
C(63)	53(4)	31(3)	30(3)	1(2)	12(3)	-1(3)
C(64)	35(3)	25(3)	27(3)	4(2)	3(2)	0(2)

Table 64. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IPr)(PPh_3)_2(CO)H_2$ **(47)**.

Atom	x	y	z	U(eq)
H(3)	3326	-638	4447	35
H(4)	5387	-844	4597	37
H(7)	1009	2851	4366	45
H(8)	-86	2311	3902	46
H(9)	565	963	3549	42
H(11)	3795	1858	4593	44
H(12A)	1664	1884	4952	72
H(12B)	2909	1689	5116	72
H(12C)	2363	823	4866	72

H(13A)	3411	3686	4481	74
H(13B)	3537	3467	4880	74
H(13C)	2286	3620	4716	74
H(14)	3361	-271	3596	46
H(15A)	1139	-1224	3679	92
H(15B)	2191	-1360	3939	92
H(15C)	2274	-1849	3564	92
H(16A)	1407	-70	3159	77
H(16B)	2594	-645	3064	77
H(16C)	2560	614	3117	77
H(19)	8537	1939	4875	49
H(20)	9924	810	4651	54
H(21)	9418	-434	4246	47
H(23)	5654	2212	4604	44
H(24A)	5393	833	5004	72
H(24B)	5121	1957	5176	72
H(24C)	6318	1372	5252	72
H(25A)	7286	3045	5083	76
H(25B)	6121	3612	4963	76
H(25C)	7174	3487	4703	76
H(26)	6589	-933	3919	46
H(27A)	7472	-2611	3945	88
H(27B)	7202	-2189	4320	88
H(27C)	8488	-2135	4174	88
H(28A)	8936	-863	3688	98
H(28B)	7934	-104	3549	98
H(28C)	7885	-1352	3476	98
H(30)	5505	-267	3596	39
H(31)	5321	-2062	3470	50
H(32)	4936	-2589	2912	55
H(33)	4805	-1328	2486	58
H(34)	5089	445	2606	46
H(36)	7344	296	2839	41
H(37)	9274	418	2689	47
H(38)	10360	1905	2845	44
H(39)	9460	3292	3144	41
H(40)	7528	3162	3290	34
H(42)	6329	2387	2526	39
H(43)	5329	3114	2070	50
H(44)	3361	3476	2120	52
H(45)	2405	3113	2634	43
H(46)	3420	2413	3091	34
H(48)	5814	4209	4308	46
H(49)	5874	5428	4752	58
H(50)	4980	7053	4697	56
H(51)	4062	7491	4190	79
H(52)	4054	6286	3740	62
H(54)	2644	3408	3692	34
H(55)	822	3905	3506	44
H(56)	587	5269	3114	50
H(57)	2221	6167	2912	51
H(58)	4032	5741	3120	43
H(60)	7024	5368	3722	38
H(61)	8501	6007	3385	44
H(62)	8377	5901	2796	53

H(63)	6751	5138	2545	46
H(64)	5302	4443	2883	35
H(65A)	1333	4888	4137	86
H(65B)	1486	5957	4357	86
H(66A)	-237	5601	3911	253
H(66B)	-174	6587	4167	253
H(67A)	-1737	4988	4196	78
H(67B)	-1618	5935	4468	78
H(68A)	-992	4709	4840	58
H(68B)	-839	3836	4543	58
H(65C)	1650	4749	4167	77
H(65D)	1997	5698	4422	77
H(66C)	366	6713	4263	109
H(66D)	778	6226	3902	109
H(67C)	-1266	5742	4095	87
H(67D)	-490	4793	3945	87
H(68C)	-1106	5157	4628	94
H(68D)	-838	4037	4448	94
H(1)	4013(18)	2140(40)	3609(10)	43(14)
H(2)	4620(30)	2890(30)	4088(7)	42(13)

Table 65. Crystal data and structure refinement for $Ru(SIPr)(PPh_3)_2(CO)H_2$ **(48)**.

Compound	$Ru(SIPr)(PPh_3)_2(CO)H_2$ **(48)**
Empirical formula	C68 H78 N2 O2 P2 Ru
Formula weight	1118.33
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_1cn$
Unit cell dimensions	a = 11.7530(1)Å $\alpha = 90^o$
	b = 12.4800(1)Å $\beta = 90^o$
	c = 39.0720(4)Å $\gamma = 90^o$
Volume	5730.98(9) $Å^3$
Z	4
Density (calculated)	1.296 Mg/m^3
Absorption coefficient	0.377 mm^{-1}
F(000)	2360
Crystal size	0.15 x 0.07 x 0.07 mm
Theta range for data collection	3.53 to 27.45 ^{o}.
Index ranges	-15<=h<=15; -16<=k<=16; -50<=l<=50
Reflections collected	83489
Independent reflections	12837 [R(int) = 0.0933]
Reflections observed (>2σ)	9950
Data Completeness	0.997
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.97 and 0.92
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12837 / 30 / 711
Goodness-of-fit on F^2	1.048
Final R indices [I>2σ(I)]	R1 = 0.0472 wR2 = 0.0757
R indices (all data)	R1 = 0.0778 wR2 = 0.0843
Absolute structure parameter	0.01(2)
Largest diff. peak and hole	0.521 and -0.508 $eÅ^{-3}$

Table 66. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIPr)(PPh_3)$_2$(CO)H_2 **(48)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	9120(1)	7657(1)	6224(1)	20(1)
P(1)	9460(1)	5871(1)	6382(1)	24(1)
P(2)	8680(1)	8378(1)	6773(1)	23(1)
O(1)	6687(2)	7117(2)	6008(1)	36(1)
O(2)	13874(3)	5261(3)	5412(1)	57(1)
N(1)	10474(2)	9432(2)	5861(1)	23(1)
N(2)	8693(2)	9577(2)	5718(1)	24(1)
C(1)	7614(3)	7371(3)	6082(1)	26(1)
C(2)	9421(3)	8994(3)	5917(1)	21(1)
C(3)	10483(3)	10281(3)	5601(1)	33(1)
C(4)	9230(4)	10515(3)	5557(1)	32(1)
C(5)	11584(3)	8962(3)	5933(1)	26(1)
C(6)	12244(3)	9380(3)	6203(1)	28(1)
C(7)	13311(3)	8914(3)	6260(1)	36(1)
C(8)	13716(3)	8092(3)	6059(1)	36(1)
C(9)	13072(3)	7727(3)	5787(1)	33(1)
C(10)	11995(3)	8156(3)	5716(1)	28(1)
C(11)	11872(3)	10345(3)	6410(1)	36(1)
C(12)	12511(4)	11368(4)	6292(1)	49(1)
C(13)	12024(4)	10183(4)	6794(1)	47(1)
C(14)	11380(3)	7806(3)	5394(1)	35(1)
C(15)	11994(4)	8241(4)	5077(1)	49(1)
C(16)	11278(3)	6587(3)	5361(1)	44(1)
C(17)	7517(3)	9379(3)	5627(1)	27(1)
C(18)	7283(3)	8630(3)	5370(1)	31(1)
C(19)	6153(3)	8527(3)	5263(1)	37(1)
C(20)	5295(3)	9145(3)	5399(1)	40(1)
C(21)	5554(3)	9894(4)	5646(1)	38(1)
C(22)	6662(3)	10037(3)	5763(1)	28(1)
C(23)	8175(3)	7938(3)	5207(1)	36(1)
C(24)	8718(4)	8506(4)	4903(1)	57(1)
C(25)	7740(4)	6837(4)	5092(1)	52(1)
C(26)	6879(3)	10890(3)	6033(1)	39(1)
C(27)	6637(5)	12023(4)	5904(1)	59(1)
C(28)	6203(4)	10669(5)	6354(1)	60(2)
C(29)	9486(3)	4917(3)	6016(1)	26(1)
C(30)	8779(4)	5067(3)	5740(1)	43(1)
C(31)	8769(4)	4367(3)	5465(1)	46(1)
C(32)	9488(4)	3512(3)	5459(1)	43(1)
C(33)	10207(4)	3344(4)	5725(1)	55(1)
C(34)	10198(4)	4049(3)	6005(1)	45(1)
C(35)	8424(3)	5183(3)	6664(1)	27(1)
C(36)	7469(3)	4685(3)	6528(1)	34(1)
C(37)	6612(3)	4313(3)	6738(1)	40(1)
C(38)	6694(4)	4418(3)	7091(1)	43(1)
C(39)	7640(4)	4884(3)	7228(1)	37(1)
C(40)	8505(3)	5269(3)	7019(1)	32(1)
C(41)	10844(3)	5516(3)	6575(1)	26(1)
C(42)	11010(3)	4666(3)	6797(1)	38(1)

C(43)	12071(4)	4390(4)	6919(1)	44(1)
C(44)	13014(4)	4967(4)	6812(1)	45(1)
C(45)	12870(3)	5812(4)	6587(1)	41(1)
C(46)	11790(3)	6088(3)	6471(1)	30(1)
C(48)	6555(3)	7414(3)	6829(1)	31(1)
C(49)	5415(3)	7327(3)	6910(1)	40(1)
C(50)	4861(3)	8152(3)	7079(1)	39(1)
C(51)	5470(3)	9043(3)	7175(1)	42(1)
C(52)	6619(3)	9126(3)	7094(1)	35(1)
C(53)	7177(3)	8319(3)	6913(1)	25(1)
C(54)	9402(3)	7751(3)	7143(1)	27(1)
C(55)	8873(3)	7519(3)	7454(1)	34(1)
C(56)	9466(4)	7089(3)	7726(1)	43(1)
C(57)	10616(4)	6879(3)	7691(1)	44(1)
C(58)	11158(4)	7100(3)	7386(1)	38(1)
C(59)	10560(3)	7531(3)	7113(1)	31(1)
C(60)	9013(4)	9790(2)	6880(1)	25(1)
C(61)	9165(4)	10148(3)	7212(1)	37(1)
C(62)	9282(4)	11222(3)	7285(1)	48(1)
C(63)	9253(5)	11969(3)	7025(1)	47(1)
C(64)	9126(4)	11633(3)	6692(1)	41(1)
C(65)	9015(4)	10552(3)	6622(1)	30(1)
C(67)	13422(6)	4734(5)	5702(2)	81(2)
C(68)	14636(11)	4564(13)	5907(3)	64(4)
C(69)	15629(10)	4569(9)	5641(3)	52(3)
C(70)	15064(4)	5377(5)	5454(2)	70(2)
C(68A)	14137(11)	3999(7)	5869(3)	79(3)
C(69A)	15184(11)	4744(10)	5801(4)	78(4)

Table 67. Bond lengths [Å] and angles [°] for $Ru(SIPr)(PPh_3)_2(CO)H_2$ **(48)**.

Ru(1)-H(2)	1.599(5)	C(26)-C(28)	1.512(6)
Ru(1)-H(1)	1.600(5)	C(26)-C(27)	1.528(6)
Ru(1)-C(1)	1.889(4)	C(29)-C(34)	1.370(5)
Ru(1)-C(2)	2.085(3)	C(29)-C(30)	1.374(5)
Ru(1)-P(1)	2.3473(9)	C(30)-C(31)	1.385(5)
Ru(1)-P(2)	2.3850(9)	C(31)-C(32)	1.361(5)
P(1)-C(41)	1.848(4)	C(32)-C(33)	1.354(6)
P(1)-C(35)	1.855(4)	C(33)-C(34)	1.405(6)
P(1)-C(29)	1.859(4)	C(35)-C(36)	1.390(5)
P(2)-C(54)	1.847(3)	C(35)-C(40)	1.395(5)
P(2)-C(53)	1.850(3)	C(36)-C(37)	1.382(5)
P(2)-C(60)	1.853(3)	C(37)-C(38)	1.387(6)
O(1)-C(1)	1.171(4)	C(38)-C(39)	1.364(6)
O(2)-C(67)	1.413(6)	C(39)-C(40)	1.389(5)
O(2)-C(70)	1.416(6)	C(41)-C(46)	1.382(5)
N(1)-C(2)	1.371(4)	C(41)-C(42)	1.386(5)
N(1)-C(5)	1.457(4)	C(42)-C(43)	1.379(5)
N(1)-C(3)	1.469(4)	C(43)-C(44)	1.386(6)
N(2)-C(2)	1.366(4)	C(44)-C(45)	1.385(6)
N(2)-C(17)	1.448(4)	C(45)-C(46)	1.390(5)
N(2)-C(4)	1.471(4)	C(48)-C(49)	1.381(5)
C(3)-C(4)	1.511(5)	C(48)-C(53)	1.385(5)
C(5)-C(10)	1.402(5)	C(49)-C(50)	1.386(6)
C(5)-C(6)	1.409(5)	C(50)-C(51)	1.374(6)

C(6)-C(7)	1.400(5)	C(51)-C(52)	1.392(5)
C(6)-C(11)	1.515(5)	C(52)-C(53)	1.393(5)
C(7)-C(8)	1.378(5)	C(54)-C(59)	1.394(5)
C(8)-C(9)	1.382(5)	C(54)-C(55)	1.396(5)
C(9)-C(10)	1.402(5)	C(55)-C(56)	1.379(5)
C(10)-C(14)	1.513(5)	C(56)-C(57)	1.383(6)
C(11)-C(13)	1.523(6)	C(57)-C(58)	1.381(6)
C(11)-C(12)	1.552(6)	C(58)-C(59)	1.384(5)
C(14)-C(16)	1.533(6)	C(60)-C(61)	1.384(4)
C(14)-C(15)	1.533(5)	C(60)-C(65)	1.385(4)
C(17)-C(18)	1.401(5)	C(61)-C(62)	1.377(5)
C(17)-C(22)	1.402(5)	C(62)-C(63)	1.379(5)
C(18)-C(19)	1.396(5)	C(63)-C(64)	1.375(5)
C(18)-C(23)	1.499(5)	C(64)-C(65)	1.383(4)
C(19)-C(20)	1.376(6)	C(67)-C(68A)	1.404(10)
C(20)-C(21)	1.377(6)	C(67)-C(68)	1.650(13)
C(21)-C(22)	1.391(5)	C(68)-C(69)	1.563(13)
C(22)-C(26)	1.519(5)	C(69)-C(70)	1.409(11)
C(23)-C(24)	1.525(6)	C(70)-C(69A)	1.574(12)
C(23)-C(25)	1.533(6)	C(68A)-C(69A)	1.564(14)
H(2)-Ru(1)-H(1)	85.5(16)	C(21)-C(22)-C(17)	118.1(4)
H(2)-Ru(1)-C(1)	177.0(12)	C(21)-C(22)-C(26)	118.4(4)
H(1)-Ru(1)-C(1)	94.2(11)	C(17)-C(22)-C(26)	123.5(3)
H(2)-Ru(1)-C(2)	84.7(11)	C(18)-C(23)-C(24)	110.8(3)
H(1)-Ru(1)-C(2)	77.6(11)	C(18)-C(23)-C(25)	114.0(3)
C(1)-Ru(1)-C(2)	98.12(13)	C(24)-C(23)-C(25)	109.1(4)
H(2)-Ru(1)-P(1)	83.8(11)	C(28)-C(26)-C(22)	111.1(4)
H(1)-Ru(1)-P(1)	76.0(11)	C(28)-C(26)-C(27)	110.1(4)
C(1)-Ru(1)-P(1)	93.27(11)	C(22)-C(26)-C(27)	112.9(3)
C(2)-Ru(1)-P(1)	151.87(9)	C(34)-C(29)-C(30)	116.9(4)
H(2)-Ru(1)-P(2)	82.5(12)	C(34)-C(29)-P(1)	122.7(3)
H(1)-Ru(1)-P(2)	167.4(11)	C(30)-C(29)-P(1)	120.4(3)
C(1)-Ru(1)-P(2)	97.63(11)	C(29)-C(30)-C(31)	122.0(4)
C(2)-Ru(1)-P(2)	104.69(9)	C(32)-C(31)-C(30)	120.0(4)
P(1)-Ru(1)-P(2)	99.14(3)	C(33)-C(32)-C(31)	119.8(4)
C(41)-P(1)-C(35)	102.91(17)	C(32)-C(33)-C(34)	119.7(4)
C(41)-P(1)-C(29)	98.42(16)	C(29)-C(34)-C(33)	121.6(4)
C(35)-P(1)-C(29)	99.91(16)	C(36)-C(35)-C(40)	118.1(4)
C(41)-P(1)-Ru(1)	119.00(13)	C(36)-C(35)-P(1)	120.5(3)
C(35)-P(1)-Ru(1)	118.95(12)	C(40)-C(35)-P(1)	120.8(3)
C(29)-P(1)-Ru(1)	114.17(11)	C(37)-C(36)-C(35)	120.7(4)
C(54)-P(2)-C(53)	101.00(15)	C(36)-C(37)-C(38)	120.6(4)
C(54)-P(2)-C(60)	97.47(15)	C(39)-C(38)-C(37)	119.2(4)
C(53)-P(2)-C(60)	99.97(17)	C(38)-C(39)-C(40)	120.9(4)
C(54)-P(2)-Ru(1)	116.34(11)	C(39)-C(40)-C(35)	120.5(4)
C(53)-P(2)-Ru(1)	117.29(12)	C(46)-C(41)-C(42)	117.9(3)
C(60)-P(2)-Ru(1)	121.01(11)	C(46)-C(41)-P(1)	117.7(3)
C(67)-O(2)-C(70)	109.0(4)	C(42)-C(41)-P(1)	124.3(3)
C(2)-N(1)-C(5)	128.1(3)	C(43)-C(42)-C(41)	122.4(4)
C(2)-N(1)-C(3)	113.8(3)	C(42)-C(43)-C(44)	119.3(4)
C(5)-N(1)-C(3)	114.7(3)	C(43)-C(44)-C(45)	119.4(4)
C(2)-N(2)-C(17)	130.3(3)	C(44)-C(45)-C(46)	120.5(4)
C(2)-N(2)-C(4)	113.4(3)	C(41)-C(46)-C(45)	120.7(4)
C(17)-N(2)-C(4)	116.2(3)	C(49)-C(48)-C(53)	121.4(4)

O(1)-C(1)-Ru(1)	174.6(3)	C(48)-C(49)-C(50)	120.5(4)
N(2)-C(2)-N(1)	105.3(3)	C(51)-C(50)-C(49)	119.1(4)
N(2)-C(2)-Ru(1)	130.3(2)	C(50)-C(51)-C(52)	120.3(4)
N(1)-C(2)-Ru(1)	124.3(2)	C(51)-C(52)-C(53)	121.2(4)
N(1)-C(3)-C(4)	102.1(3)	C(48)-C(53)-C(52)	117.5(3)
N(2)-C(4)-C(3)	102.5(3)	C(48)-C(53)-P(2)	117.7(3)
C(10)-C(5)-C(6)	122.0(3)	C(52)-C(53)-P(2)	124.8(3)
C(10)-C(5)-N(1)	118.7(3)	C(59)-C(54)-C(55)	117.7(3)
C(6)-C(5)-N(1)	119.2(3)	C(59)-C(54)-P(2)	117.9(3)
C(7)-C(6)-C(5)	117.3(4)	C(55)-C(54)-P(2)	124.3(3)
C(7)-C(6)-C(11)	120.2(3)	C(56)-C(55)-C(54)	121.8(4)
C(5)-C(6)-C(11)	122.4(3)	C(55)-C(56)-C(57)	119.5(4)
C(8)-C(7)-C(6)	121.8(4)	C(58)-C(57)-C(56)	119.7(4)
C(7)-C(8)-C(9)	119.7(4)	C(57)-C(58)-C(59)	120.6(4)
C(8)-C(9)-C(10)	121.3(4)	C(58)-C(59)-C(54)	120.6(4)
C(5)-C(10)-C(9)	117.8(3)	C(61)-C(60)-C(65)	117.4(3)
C(5)-C(10)-C(14)	123.0(3)	C(61)-C(60)-P(2)	123.0(2)
C(9)-C(10)-C(14)	119.0(3)	C(65)-C(60)-P(2)	119.3(2)
C(6)-C(11)-C(13)	112.7(4)	C(62)-C(61)-C(60)	121.4(3)
C(6)-C(11)-C(12)	110.8(3)	C(61)-C(62)-C(63)	120.2(4)
C(13)-C(11)-C(12)	110.2(4)	C(64)-C(63)-C(62)	119.6(3)
C(10)-C(14)-C(16)	113.2(3)	C(63)-C(64)-C(65)	119.6(3)
C(10)-C(14)-C(15)	110.1(3)	C(64)-C(65)-C(60)	121.8(3)
C(16)-C(14)-C(15)	108.6(3)	C(68A)-C(67)-O(2)	116.8(7)
C(18)-C(17)-C(22)	121.4(3)	C(68A)-C(67)-C(68)	34.2(6)
C(18)-C(17)-N(2)	118.5(3)	O(2)-C(67)-C(68)	97.1(6)
C(22)-C(17)-N(2)	119.4(3)	C(69)-C(68)-C(67)	108.7(9)
C(19)-C(18)-C(17)	117.5(4)	C(70)-C(69)-C(68)	89.8(8)
C(19)-C(18)-C(23)	119.1(4)	C(69)-C(70)-O(2)	116.9(7)
C(17)-C(18)-C(23)	123.4(3)	C(69)-C(70)-C(69A)	32.3(6)
C(20)-C(19)-C(18)	122.1(4)	O(2)-C(70)-C(69A)	97.9(6)
C(19)-C(20)-C(21)	119.2(4)	C(67)-C(68A)-C(69A)	90.2(7)
C(20)-C(21)-C(22)	121.7(4)	C(68A)-C(69A)-C(70)	111.9(9)

Table 68. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(SIPr)(PPh_3)_2(CO)H_2$ **(48)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	23(1)	20(1)	17(1)	1(1)	1(1)	0(1)
P(1)	28(1)	23(1)	21(1)	1(1)	0(1)	0(1)
P(2)	28(1)	21(1)	19(1)	0(1)	2(1)	0(1)
O(1)	27(2)	45(2)	35(2)	2(1)	-5(1)	-9(1)
O(2)	54(2)	73(2)	45(2)	0(2)	-1(2)	-2(2)
N(1)	25(2)	24(2)	21(2)	6(1)	0(1)	-2(1)
N(2)	26(2)	24(2)	23(2)	8(1)	-2(1)	-2(1)
C(1)	35(2)	21(2)	21(2)	5(2)	-1(2)	3(2)
C(2)	25(2)	21(2)	17(2)	-5(1)	-3(1)	1(1)
C(3)	29(2)	35(2)	36(2)	15(2)	0(2)	-6(2)
C(4)	32(2)	31(2)	33(2)	10(2)	-3(2)	-3(2)
C(5)	28(2)	28(2)	21(2)	7(2)	0(2)	-3(2)
C(6)	26(2)	32(2)	27(2)	4(2)	1(2)	-4(2)
C(7)	26(2)	48(3)	34(2)	8(2)	-5(2)	-8(2)
C(8)	27(2)	43(2)	38(2)	10(2)	3(2)	4(2)

C(9)	31(2)	34(2)	33(2)	2(2)	7(2)	3(2)
C(10)	26(2)	30(2)	27(2)	6(2)	6(2)	-3(2)
C(11)	29(2)	42(3)	36(3)	-11(2)	-5(2)	0(2)
C(12)	57(3)	42(3)	49(3)	-3(2)	-5(2)	-6(2)
C(13)	47(3)	59(3)	35(3)	-11(2)	-2(2)	-10(2)
C(14)	30(2)	50(3)	23(2)	-4(2)	3(2)	0(2)
C(15)	50(3)	65(3)	33(3)	2(2)	9(2)	1(2)
C(16)	37(2)	53(3)	43(3)	-15(2)	5(2)	-2(2)
C(17)	26(2)	30(2)	25(2)	13(2)	-3(2)	0(2)
C(18)	28(2)	34(2)	30(2)	9(2)	-5(2)	-2(2)
C(19)	40(2)	34(2)	38(3)	9(2)	-12(2)	-6(2)
C(20)	29(2)	51(3)	39(2)	18(2)	-9(2)	-7(2)
C(21)	26(2)	55(3)	32(2)	13(2)	3(2)	5(2)
C(22)	28(2)	29(2)	27(2)	12(2)	0(2)	-1(2)
C(23)	41(2)	33(2)	34(2)	-6(2)	-8(2)	-3(2)
C(24)	58(3)	59(3)	53(3)	-1(2)	20(2)	4(2)
C(25)	70(3)	44(3)	42(3)	-5(2)	-4(2)	5(2)
C(26)	36(2)	51(3)	31(2)	3(2)	0(2)	14(2)
C(27)	86(4)	42(3)	51(3)	-6(2)	-10(3)	13(3)
C(28)	49(3)	106(5)	25(3)	1(3)	4(2)	6(3)
C(29)	34(2)	20(2)	25(2)	4(2)	3(2)	-2(2)
C(30)	61(3)	33(2)	35(2)	-1(2)	-8(2)	14(2)
C(31)	73(4)	37(2)	29(2)	-7(2)	-9(2)	2(2)
C(32)	55(3)	33(2)	42(3)	-17(2)	16(2)	-11(2)
C(33)	46(3)	36(3)	82(4)	-22(3)	-11(3)	14(2)
C(34)	51(3)	37(2)	48(3)	-13(2)	-16(2)	9(2)
C(35)	37(2)	18(2)	26(2)	2(2)	4(2)	0(2)
C(36)	38(2)	30(2)	34(2)	1(2)	3(2)	-5(2)
C(37)	34(2)	40(3)	46(3)	2(2)	5(2)	-14(2)
C(38)	45(3)	37(3)	46(3)	7(2)	20(2)	-7(2)
C(39)	54(3)	27(2)	30(2)	1(2)	10(2)	-3(2)
C(40)	41(2)	26(2)	27(2)	6(2)	2(2)	0(2)
C(41)	28(2)	27(2)	24(2)	0(2)	-3(2)	6(2)
C(42)	34(2)	39(3)	42(3)	10(2)	0(2)	5(2)
C(43)	48(3)	48(3)	36(3)	16(2)	-7(2)	15(2)
C(44)	33(2)	57(3)	46(3)	1(2)	-10(2)	12(2)
C(45)	30(2)	52(3)	42(3)	-3(2)	-5(2)	0(2)
C(46)	30(2)	32(2)	28(2)	1(2)	-1(2)	4(2)
C(48)	37(2)	29(2)	26(2)	3(2)	3(2)	-6(2)
C(49)	36(2)	43(3)	40(2)	6(2)	1(2)	-12(2)
C(50)	24(2)	49(3)	46(3)	14(2)	10(2)	5(2)
C(51)	41(3)	38(3)	48(3)	3(2)	20(2)	9(2)
C(52)	37(2)	30(2)	38(2)	-4(2)	8(2)	-4(2)
C(53)	27(2)	29(2)	18(2)	3(2)	2(2)	-1(2)
C(54)	39(3)	20(2)	22(2)	-3(1)	-2(1)	2(2)
C(55)	51(3)	26(2)	25(2)	-2(2)	1(2)	1(2)
C(56)	76(4)	29(2)	24(2)	6(2)	-2(2)	-1(2)
C(57)	79(3)	27(2)	26(2)	6(2)	-19(2)	4(2)
C(58)	47(3)	31(2)	36(2)	-4(2)	-16(2)	4(2)
C(59)	42(2)	28(2)	24(2)	-1(2)	-6(2)	2(2)
C(60)	31(2)	24(2)	22(2)	-2(1)	2(2)	0(2)
C(61)	55(2)	28(2)	27(2)	0(1)	-5(2)	-4(3)
C(62)	68(3)	39(2)	37(2)	-12(2)	-2(3)	-13(3)
C(63)	67(3)	25(2)	47(2)	-7(2)	9(3)	-7(2)
C(64)	57(2)	25(2)	41(2)	5(2)	3(3)	0(3)

C(65)	33(2)	28(2)	28(2)	0(1)	2(2)	-3(2)
C(67)	124(6)	65(4)	54(4)	-2(3)	15(4)	-10(4)
C(68)	81(8)	63(8)	49(6)	21(6)	23(6)	20(7)
C(69)	51(6)	50(6)	54(6)	4(5)	-3(5)	19(5)
C(70)	50(3)	73(4)	85(4)	-25(3)	-13(3)	6(3)
C(68A)	97(7)	49(5)	92(6)	6(5)	-14(7)	0(6)
C(69A)	54(7)	64(7)	116(9)	-9(7)	-22(6)	9(6)

Table 69. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(SIPr)(PPh_3)$_2$(CO)H_2 **(48)**.

Atom	x	y	z	U(eq)
H(3A)	10826	10027	5384	40
H(3B)	10902	10921	5682	40
H(4A)	9013	11186	5676	38
H(4B)	9022	10572	5313	38
H(7)	13768	9172	6443	43
H(8)	14435	7778	6106	43
H(9)	13365	7173	5645	39
H(11)	11043	10460	6366	43
H(12A)	13318	11309	6353	74
H(12B)	12181	11997	6405	74
H(12C)	12439	11446	6044	74
H(13A)	12838	10142	6848	70
H(13B)	11651	9515	6863	70
H(13C)	11683	10786	6917	70
H(14)	10595	8116	5399	42
H(15A)	11553	8065	4872	74
H(15B)	12751	7916	5061	74
H(15C)	12070	9021	5096	74
H(16A)	10937	6292	5570	66
H(16B)	12036	6276	5328	66
H(16C)	10797	6412	5164	66
H(19)	5972	8015	5092	45
H(20)	4532	9055	5324	47
H(21)	4962	10323	5738	45
H(23)	8784	7815	5382	43
H(24A)	9044	9189	4978	85
H(24B)	8139	8640	4728	85
H(24C)	9321	8054	4807	85
H(25A)	7217	6926	4899	78
H(25B)	7339	6491	5282	78
H(25C)	8385	6391	5022	78
H(26)	7704	10855	6094	47
H(27A)	6821	12541	6084	89
H(27B)	5831	12086	5844	89
H(27C)	7105	12170	5702	89
H(28A)	6288	9914	6418	91
H(28B)	5398	10827	6313	91
H(28C)	6486	11123	6540	91
H(30)	8283	5667	5738	52
H(31)	8261	4485	5279	55
H(32)	9485	3035	5270	52
H(33)	10716	2753	5721	66

H(34)	10697	3919	6192	54
H(36)	7406	4599	6287	41
H(37)	5960	3982	6641	48
H(38)	6099	4169	7235	51
H(39)	7708	4945	7469	44
H(40)	9157	5593	7119	38
H(42)	10369	4258	6868	46
H(43)	12155	3810	7075	53
H(44)	13751	4785	6893	54
H(45)	13514	6204	6510	49
H(46)	11702	6677	6319	36
H(48)	6921	6840	6713	37
H(49)	5009	6697	6850	48
H(50)	4070	8102	7128	47
H(51)	5105	9603	7297	51
H(52)	7031	9745	7162	42
H(55)	8084	7661	7479	41
H(56)	9087	6938	7935	52
H(57)	11031	6583	7877	53
H(58)	11947	6956	7362	46
H(59)	10944	7679	6904	38
H(61)	9188	9643	7394	44
H(62)	9383	11450	7515	57
H(63)	9320	12711	7075	56
H(64)	9114	12141	6511	49
H(65)	8939	10325	6391	36
H(67A)	13055	4045	5642	97
H(67B)	12883	5190	5831	97
H(68A)	14747	5149	6075	77
H(68B)	14626	3874	6032	77
H(69A)	16368	4800	5737	62
H(69B)	15709	3886	5514	62
H(70A)	15415	5417	5224	84
H(70B)	15208	6070	5570	84
H(68C)	14188	3297	5752	95
H(68D)	13958	3906	6115	95
H(69C)	15884	4304	5794	94
H(69D)	15258	5260	5992	94
H(1)	9690(20)	7140(20)	5890(5)	28(9)
H(2)	10398(10)	7840(30)	6352(8)	21(9)

Table 70. Crystal data and structure refinement for $Ru(SIMes)(PPh_3)(CO)_3$ **(52)**.

Compound	$Ru(SIMes)(PPh_3)(CO)_3$ **(52)**
Empirical formula	C48 H47 N2 O3 P Ru
Formula weight	831.92
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P212121
Unit cell dimensions	a = 11.07800(10)Å α = 90°
	b = 12.63100(10)Å β = 90°
	c = 29.4160(3)Å γ = 90°
Volume	4116.07(6) $Å^3$
Z	4
Density (calculated)	1.342 Mg/m^3
Absorption coefficient	0.463 mm^{-1}
F(000)	1728
Crystal size	0.30 x 0.30 x 0.30 mm
Theta range for data collection	3.68 to 30.06°
Index ranges	-15<=h<=15; -17<=k<=17; -40<=l<=41
Reflections collected	60028
Independent reflections	12003 [R(int) = 0.0658]
Reflections observed (>2σ)	10017
Data Completeness	0.995
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.87 and 0.81
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12003 / 0 / 458
Goodness-of-fit on F^2	1.012
Final R indices [I>2σ(I)]	R^1 = 0.0406 wR2 = 0.0888
R indices (all data)	R^1 = 0.0580 wR2 = 0.0967
Absolute structure parameter	-0.04(2)
Largest diff. peak and hole	0.655 and -0.788 $eÅ^{-3}$

Table 71. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(SIMes)(PPh_3)(CO)_3$ **(52)**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	3059(1)	7278(1)	3318(1)	22(1)
P(1)	2359(1)	8369(1)	3903(1)	25(1)
O(1)	1434(2)	5549(2)	3721(1)	52(1)
O(2)	5585(2)	8005(2)	3616(1)	47(1)
O(3)	2068(2)	9026(2)	2697(1)	39(1)
N(1)	3023(2)	5855(2)	2454(1)	26(1)
N(2)	4628(2)	5540(2)	2856(1)	28(1)
C(43A)	2408(5)	12391(3)	5382(2)	113(10)
C(44A)	2339(4)	11709(3)	5011(1)	74(7)
C(45A)	2294(4)	12116(2)	4573(1)	77(7)
C(46A)	2318(5)	13205(2)	4504(2)	105(10)
C(47A)	2388(5)	13886(3)	4874(2)	130(13)
C(48A)	2433(5)	13479(3)	5313(2)	151(16)
C(1)	2046(2)	6186(1)	3560(1)	34(1)
C(2)	4673(2)	7659(2)	3499(1)	30(1)

C(3)	2434(2)	8317(1)	2900(1)	28(1)
C(4)	3632(1)	6158(1)	2831(1)	23(1)
C(5)	3641(2)	5034(2)	2189(1)	34(1)
C(6)	4680(3)	4718(3)	2500(1)	39(1)
C(7)	1954(3)	6321(2)	2263(1)	25(1)
C(8)	837(3)	5845(2)	2341(1)	27(1)
C(9)	-173(2)	6281(2)	2134(1)	29(1)
C(10)	-91(2)	7170(2)	1853(1)	30(1)
C(11)	1033(2)	7604(2)	1777(1)	29(1)
C(12)	2073(2)	7191(2)	1975(1)	27(1)
C(13)	712(3)	4863(2)	2629(1)	37(1)
C(14)	-1203(3)	7617(3)	1625(1)	40(1)
C(15)	3284(3)	7684(3)	1872(1)	35(1)
C(16)	5568(2)	5564(2)	3193(1)	28(1)
C(17)	6645(2)	6077(2)	3079(1)	30(1)
C(18)	7593(3)	6042(2)	3385(1)	38(1)
C(19)	7483(3)	5528(3)	3807(1)	44(1)
C(20)	6411(3)	5023(3)	3898(1)	44(1)
C(21)	5445(3)	5007(2)	3595(1)	34(1)
C(22)	6762(3)	6703(3)	2647(1)	41(1)
C(23)	8529(4)	5535(4)	4143(2)	70(1)
C(24)	4317(3)	4393(3)	3710(1)	46(1)
C(25)	2235(2)	7763(2)	4472(1)	29(1)
C(26)	2998(3)	6936(3)	4589(1)	43(1)
C(27)	2964(4)	6503(3)	5025(1)	53(1)
C(28)	2151(3)	6876(3)	5340(1)	47(1)
C(29)	1388(4)	7682(4)	5225(1)	55(1)
C(30)	1415(3)	8125(3)	4791(1)	48(1)
C(31)	865(3)	8961(2)	3831(1)	28(1)
C(32)	564(3)	9951(2)	4011(1)	35(1)
C(33)	-612(3)	10336(3)	3973(1)	41(1)
C(34)	-1487(3)	9744(3)	3765(1)	37(1)
C(35)	-1206(3)	8770(3)	3583(1)	38(1)
C(36)	-33(3)	8379(2)	3612(1)	32(1)
C(37)	3331(3)	9516(2)	4011(1)	30(1)
C(38)	3381(3)	10325(2)	3689(1)	34(1)
C(39)	4165(4)	11162(3)	3736(1)	45(1)
C(40)	4962(4)	11190(3)	4100(2)	63(1)
C(41)	4967(4)	10362(4)	4414(2)	66(1)
C(42)	4130(4)	9548(3)	4371(1)	49(1)
C(43)	2866(8)	12188(8)	4973(3)	265(9)
C(44)	1746(11)	11692(5)	4983(2)	144(4)
C(45)	741(8)	12197(7)	4801(3)	208(6)
C(46)	856(8)	13198(7)	4610(3)	160(5)
C(47)	1975(10)	13694(5)	4600(3)	143(4)
C(48)	2980(7)	13190(9)	4782(4)	229(7)

Table 72. Bond lengths [Å] and angles [°] for Ru(SIMes)(PPh_3)($CO)_3$ **(52)**.

Ru(1)-C(1)	1.9150(14)	C(16)-C(21)	1.384(4)
Ru(1)-C(2)	1.9272(15)	C(16)-C(17)	1.399(4)
Ru(1)-C(3)	1.9279(15)	C(17)-C(18)	1.384(4)
Ru(1)-C(4)	2.1117(12)	C(17)-C(22)	1.502(4)
Ru(1)-P(1)	2.3372(7)	C(18)-C(19)	1.408(5)
P(1)-C(31)	1.829(3)	C(19)-C(20)	1.375(5)

P(1)-C(37)	1.833(3)	C(19)-C(23)	1.522(5)
P(1)-C(25)	1.846(3)	C(20)-C(21)	1.393(5)
O(1)-C(1)	1.153(3)	C(21)-C(24)	1.509(5)
O(2)-C(2)	1.153(3)	C(25)-C(30)	1.383(4)
O(3)-C(3)	1.150(2)	C(25)-C(26)	1.387(4)
N(1)-C(4)	1.352(3)	C(26)-C(27)	1.396(4)
N(1)-C(7)	1.438(4)	C(27)-C(28)	1.375(5)
N(1)-C(5)	1.468(3)	C(28)-C(29)	1.366(5)
N(2)-C(4)	1.354(3)	C(29)-C(30)	1.394(5)
N(2)-C(16)	1.437(3)	C(31)-C(36)	1.394(4)
N(2)-C(6)	1.474(4)	C(31)-C(32)	1.399(4)
C(43A)-C(44A)	1.3900	C(32)-C(33)	1.395(5)
C(43A)-C(48A)	1.3900	C(33)-C(34)	1.368(5)
C(44A)-C(45A)	1.3900	C(34)-C(35)	1.378(5)
C(45A)-C(46A)	1.3900	C(35)-C(36)	1.394(4)
C(46A)-C(47A)	1.3900	C(37)-C(42)	1.381(5)
C(47A)-C(48A)	1.3900	C(37)-C(38)	1.394(4)
C(5)-C(6)	1.524(4)	C(38)-C(39)	1.375(4)
C(7)-C(12)	1.393(4)	C(39)-C(40)	1.389(6)
C(7)-C(8)	1.395(4)	C(40)-C(41)	1.394(6)
C(8)-C(9)	1.388(4)	C(41)-C(42)	1.390(5)
C(8)-C(13)	1.508(4)	C(43)-C(44)	1.3900
C(9)-C(10)	1.399(4)	C(43)-C(48)	1.3900
C(10)-C(11)	1.379(4)	C(44)-C(45)	1.3900
C(10)-C(14)	1.511(4)	C(45)-C(46)	1.3900
C(11)-C(12)	1.392(4)	C(46)-C(47)	1.3900
C(12)-C(15)	1.509(4)	C(47)-C(48)	1.3900
C(1)-Ru(1)-C(2)	128.38(8)	C(11)-C(12)-C(7)	118.1(3)
C(1)-Ru(1)-C(3)	121.17(8)	C(11)-C(12)-C(15)	119.8(2)
C(2)-Ru(1)-C(3)	109.83(7)	C(7)-C(12)-C(15)	122.1(3)
C(1)-Ru(1)-C(4)	86.90(5)	C(21)-C(16)-C(17)	121.6(3)
C(2)-Ru(1)-C(4)	94.36(6)	C(21)-C(16)-N(2)	120.5(3)
C(3)-Ru(1)-C(4)	97.47(6)	C(17)-C(16)-N(2)	117.5(3)
C(1)-Ru(1)-P(1)	87.56(5)	C(18)-C(17)-C(16)	118.5(3)
C(2)-Ru(1)-P(1)	87.50(5)	C(18)-C(17)-C(22)	120.1(3)
C(3)-Ru(1)-P(1)	87.13(5)	C(16)-C(17)-C(22)	121.4(3)
C(4)-Ru(1)-P(1)	174.11(5)	C(17)-C(18)-C(19)	121.6(3)
C(31)-P(1)-C(37)	103.24(13)	C(20)-C(19)-C(18)	117.5(3)
C(31)-P(1)-C(25)	101.98(13)	C(20)-C(19)-C(23)	122.3(4)
C(37)-P(1)-C(25)	102.42(14)	C(18)-C(19)-C(23)	120.3(3)
C(31)-P(1)-Ru(1)	117.10(10)	C(19)-C(20)-C(21)	123.1(3)
C(37)-P(1)-Ru(1)	113.49(9)	C(16)-C(21)-C(20)	117.7(3)
C(25)-P(1)-Ru(1)	116.59(10)	C(16)-C(21)-C(24)	122.3(3)
C(4)-N(1)-C(7)	128.0(2)	C(20)-C(21)-C(24)	120.0(3)
C(4)-N(1)-C(5)	113.8(2)	C(30)-C(25)-C(26)	118.8(3)
C(7)-N(1)-C(5)	117.7(2)	C(30)-C(25)-P(1)	121.8(2)
C(4)-N(2)-C(16)	128.0(2)	C(26)-C(25)-P(1)	119.4(2)
C(4)-N(2)-C(6)	113.5(2)	C(25)-C(26)-C(27)	120.4(3)
C(16)-N(2)-C(6)	118.4(2)	C(28)-C(27)-C(26)	120.2(3)
C(44A)-C(43A)-C(48A)	120.0	C(29)-C(28)-C(27)	119.6(3)
C(45A)-C(44A)-C(43A)	120.0	C(28)-C(29)-C(30)	120.8(3)
C(44A)-C(45A)-C(46A)	120.0	C(25)-C(30)-C(29)	120.1(3)
C(47A)-C(46A)-C(45A)	120.0	C(36)-C(31)-C(32)	118.5(3)
C(46A)-C(47A)-C(48A)	120.0	C(36)-C(31)-P(1)	118.9(2)

C(47A)-C(48A)-C(43A)	120.0	C(32)-C(31)-P(1)	122.5(2)
O(1)-C(1)-Ru(1)	177.36(19)	C(33)-C(32)-C(31)	120.2(3)
O(2)-C(2)-Ru(1)	171.99(19)	C(34)-C(33)-C(32)	120.5(3)
O(3)-C(3)-Ru(1)	171.00(17)	C(33)-C(34)-C(35)	120.1(3)
N(1)-C(4)-N(2)	106.74(16)	C(34)-C(35)-C(36)	120.2(3)
N(1)-C(4)-Ru(1)	126.54(13)	C(35)-C(36)-C(31)	120.5(3)
N(2)-C(4)-Ru(1)	126.49(13)	C(42)-C(37)-C(38)	118.3(3)
N(1)-C(5)-C(6)	102.55(17)	C(42)-C(37)-P(1)	122.1(2)
N(2)-C(6)-C(5)	102.3(2)	C(38)-C(37)-P(1)	119.0(2)
C(12)-C(7)-C(8)	121.7(3)	C(39)-C(38)-C(37)	121.4(3)
C(12)-C(7)-N(1)	118.9(3)	C(38)-C(39)-C(40)	119.8(3)
C(8)-C(7)-N(1)	119.3(2)	C(39)-C(40)-C(41)	119.7(4)
C(9)-C(8)-C(7)	118.1(3)	C(42)-C(41)-C(40)	119.5(4)
C(9)-C(8)-C(13)	119.9(3)	C(37)-C(42)-C(41)	121.2(3)
C(7)-C(8)-C(13)	121.9(3)	C(44)-C(43)-C(48)	120.0
C(8)-C(9)-C(10)	121.8(3)	C(43)-C(44)-C(45)	120.0
C(11)-C(10)-C(9)	118.2(3)	C(44)-C(45)-C(46)	120.0
C(11)-C(10)-C(14)	121.1(3)	C(47)-C(46)-C(45)	120.0
C(9)-C(10)-C(14)	120.7(3)	C(48)-C(47)-C(46)	120.0
C(10)-C(11)-C(12)	122.1(3)	C(47)-C(48)-C(43)	120.0

Table 73. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(SIMes)(PPh_3)(CO)_3$ **(52)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	22(1)	19(1)	26(1)	-1(1)	1(1)	1(1)
P(1)	28(1)	21(1)	26(1)	0(1)	1(1)	2(1)
O(1)	53(1)	37(1)	64(2)	-2(1)	23(1)	-14(1)
O(2)	28(1)	50(2)	64(2)	-26(1)	-5(1)	0(1)
O(3)	50(1)	30(1)	36(1)	0(1)	-4(1)	13(1)
N(1)	23(1)	21(1)	35(1)	-7(1)	-3(1)	3(1)
N(2)	26(1)	25(1)	34(1)	-7(1)	-6(1)	7(1)
C(1)	35(2)	25(1)	43(2)	-6(1)	10(1)	0(1)
C(2)	29(1)	29(1)	32(1)	-8(1)	3(1)	4(1)
C(3)	29(1)	26(1)	30(1)	-8(1)	1(1)	2(1)
C(4)	21(1)	16(1)	32(1)	-2(1)	2(1)	-1(1)
C(5)	30(2)	29(2)	42(2)	-13(1)	-4(1)	6(1)
C(6)	34(2)	30(2)	52(2)	-18(1)	-8(2)	9(1)
C(7)	25(1)	21(1)	30(1)	-5(1)	-5(1)	1(1)
C(8)	27(1)	25(1)	30(1)	-2(1)	-3(1)	0(1)
C(9)	23(1)	27(1)	36(2)	-3(1)	-3(1)	-2(1)
C(10)	32(1)	26(1)	31(1)	-6(1)	-4(1)	3(1)
C(11)	37(1)	20(1)	28(1)	-1(1)	-2(1)	-1(1)
C(12)	28(1)	22(1)	30(1)	-3(1)	2(1)	-2(1)
C(13)	32(2)	34(2)	44(2)	7(1)	-5(1)	-6(1)
C(14)	38(2)	36(2)	45(2)	-1(2)	-15(1)	4(1)
C(15)	32(2)	32(1)	41(2)	-5(1)	6(1)	-8(1)
C(16)	23(1)	22(1)	39(2)	-5(1)	-4(1)	6(1)
C(17)	27(1)	25(1)	38(2)	-4(1)	2(1)	4(1)
C(18)	23(1)	39(2)	52(2)	-5(2)	-3(1)	5(1)
C(19)	35(2)	53(2)	44(2)	-7(2)	-11(2)	8(2)
C(20)	45(2)	52(2)	36(2)	7(2)	-3(2)	10(2)
C(21)	30(2)	30(2)	41(2)	0(1)	1(1)	7(1)

C(22)	34(2)	41(2)	46(2)	3(1)	7(1)	1(1)
C(23)	50(2)	96(4)	62(3)	-5(3)	-24(2)	9(2)
C(24)	38(2)	41(2)	59(2)	13(2)	4(2)	2(2)
C(25)	34(1)	28(1)	27(1)	3(1)	1(1)	-2(1)
C(26)	42(2)	45(2)	40(2)	13(1)	6(2)	12(2)
C(27)	56(2)	55(2)	48(2)	19(2)	-4(2)	10(2)
C(28)	48(2)	63(2)	30(2)	17(2)	-1(1)	-3(2)
C(29)	56(2)	77(3)	33(2)	8(2)	11(2)	13(2)
C(30)	54(2)	59(2)	31(2)	9(2)	9(2)	21(2)
C(31)	31(1)	26(1)	28(1)	3(1)	6(1)	4(1)
C(32)	38(2)	29(2)	37(2)	-1(1)	3(1)	5(1)
C(33)	48(2)	35(2)	40(2)	5(1)	7(2)	17(2)
C(34)	35(2)	43(2)	34(2)	9(1)	5(1)	13(1)
C(35)	32(2)	41(2)	41(2)	5(1)	0(1)	5(1)
C(36)	32(2)	30(2)	34(2)	2(1)	1(1)	6(1)
C(37)	35(2)	25(1)	30(1)	-4(1)	3(1)	0(1)
C(38)	38(2)	29(2)	35(2)	0(1)	2(1)	-2(1)
C(39)	58(2)	32(2)	46(2)	-1(1)	2(2)	-8(2)
C(40)	80(3)	45(2)	63(3)	-4(2)	-5(2)	-29(2)
C(41)	83(3)	59(3)	55(3)	-2(2)	-26(2)	-25(2)
C(42)	69(2)	38(2)	40(2)	0(2)	-15(2)	-12(2)

Table 74. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(SIMes)(PPh_3)$(CO)_3$ **(52)**.

Atom	x	y	z	U(eq)
H(43A)	2439	12112	5681	135
H(44A)	2322	10965	5058	88
H(45A)	2246	11651	4320	93
H(46A)	2288	13483	4204	127
H(47A)	2405	14630	4828	156
H(48A)	2480	13945	5566	181
H(5A)	3942	5319	1897	40
H(5B)	3100	4426	2128	40
H(6A)	4553	4003	2630	46
H(6B)	5461	4734	2337	46
H(9)	-940	5967	2185	34
H(11)	1100	8204	1584	34
H(13A)	657	4240	2431	55
H(13B)	-19	4915	2815	55
H(13C)	1419	4795	2827	55
H(14A)	-1440	7157	1372	60
H(14B)	-1026	8328	1509	60
H(14C)	-1863	7656	1846	60
H(15A)	3188	8450	1833	53
H(15B)	3612	7376	1593	53
H(15C)	3840	7546	2125	53
H(18)	8335	6373	3308	45
H(20)	6324	4669	4181	53
H(22A)	6095	7210	2625	61
H(22B)	6738	6222	2386	61
H(22C)	7531	7087	2648	61
H(23A)	8351	5053	4395	104
H(23B)	8643	6253	4260	104

H(23C)	9267	5303	3988	104
H(24A)	3773	4840	3889	69
H(24B)	4534	3763	3887	69
H(24C)	3913	4175	3429	69
H(26)	3547	6662	4370	51
H(27)	3505	5950	5105	63
H(28)	2120	6575	5635	57
H(29)	832	7945	5443	66
H(30)	869	8676	4714	58
H(32)	1162	10363	4160	42
H(33)	-807	11013	4092	49
H(34)	-2290	10006	3745	44
H(35)	-1815	8362	3437	45
H(36)	157	7711	3482	38
H(38)	2862	10298	3432	40
H(39)	4163	11720	3519	54
H(40)	5500	11769	4136	75
H(41)	5538	10354	4655	79
H(42)	4107	9004	4594	59
H(43)	3553	11843	5097	318
H(44)	1668	11008	5113	173
H(45)	-24	11857	4807	249
H(46)	169	13543	4485	192
H(47)	2053	14379	4469	171
H(48)	3745	13529	4775	274

Table 75. Crystal data and structure refinement for $Ru(IPr)(PPh_3)(CO)_3$ **(53)**.

Compound	$Ru(IPr)(PPh_3)(CO)_3$ **(53)**
Empirical formula	C48 H51 N2 O3 P Ru
Formula weight	835.95
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 15.1130 (1)Å α = 90°
	b = 16.9900(1)Å β = 90°
	c = 33.3570(3)Å γ = 90°
Volume	8565.07(11) $Å^3$
Z	8
Density (calculated)	1.297 Mg/m^3
Absorption coefficient	0.446 mm^{-1}
F(000)	3488
Crystal size	0.60 x 0.60 x 0.50 mm
Theta range for data collection	3.55 to 30.00°
Index ranges	-20<=h<=21; -23<=k<=23; -46<=l<=46
Reflections collected	70939
Independent reflections	12416 [R(int) = 0.0635]
Reflections observed (>2σ)	8996
Data Completeness	0.994
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.82 and 0.74
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12416 / 0 / 504
Goodness-of-fit on F^2	1.014
Final R indices [I>2σ(I)]	R1 = 0.0368 wR2 = 0.0762
R indices (all data)	R1 = 0.0647 wR2 = 0.0861
Largest diff. peak and hole	0.768 and -0.977 $eÅ^{-3}$

Table 76. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IPr)(PPh_3)(CO)_3$ **(53)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	-680(1)	2162(1)	8758(1)	17(1)
P(1)	207(1)	1057(1)	8652(1)	18(1)
O(1)	199(1)	2117(1)	9587(1)	34(1)
O(2)	-2163(1)	1029(1)	8497(1)	43(1)
O(3)	471(1)	2939(1)	8111(1)	31(1)
N(1)	-2209(1)	3414(1)	8613(1)	18(1)
N(2)	-1317(1)	3826(1)	9068(1)	19(1)
C(1)	-189(1)	2183(1)	9290(1)	24(1)
C(2)	-1653(1)	1497(1)	8599(1)	28(1)
C(3)	13(1)	2679(1)	8353(1)	22(1)
C(4)	-1479(1)	3184(1)	8828(1)	17(1)
C(5)	-2473(1)	4175(1)	8711(1)	22(1)
C(6)	-1919(1)	4430(1)	8997(1)	22(1)
C(7)	-2719(1)	2935(1)	8339(1)	20(1)
C(8)	-3481(1)	2562(1)	8489(1)	24(1)
C(9)	-3950(1)	2087(1)	8221(1)	31(1)

C(10)	-3693(2)	2017(1)	7826(1)	36(1)
C(11)	-2974(1)	2429(1)	7681(1)	32(1)
C(12)	-2466(1)	2901(1)	7936(1)	23(1)
C(13)	-3789(1)	2662(1)	8919(1)	29(1)
C(14)	-3355(2)	2065(1)	9202(1)	38(1)
C(15)	-4803(2)	2614(1)	8961(1)	41(1)
C(16)	-1688(1)	3369(1)	7774(1)	26(1)
C(17)	-1181(2)	2916(1)	7451(1)	39(1)
C(18)	-1992(2)	4172(1)	7612(1)	44(1)
C(19)	-670(1)	3882(1)	9384(1)	21(1)
C(20)	182(1)	4153(1)	9290(1)	24(1)
C(21)	780(1)	4226(1)	9606(1)	31(1)
C(22)	536(2)	4050(1)	9995(1)	36(1)
C(23)	-310(2)	3790(1)	10080(1)	32(1)
C(24)	-938(1)	3699(1)	9775(1)	25(1)
C(25)	432(1)	4388(1)	8865(1)	27(1)
C(26)	1395(2)	4197(2)	8759(1)	42(1)
C(27)	242(2)	5265(1)	8798(1)	38(1)
C(28)	-1869(1)	3418(1)	9878(1)	29(1)
C(29)	-2344(2)	4002(1)	10154(1)	42(1)
C(30)	-1859(2)	2597(1)	10071(1)	41(1)
C(31)	1371(1)	1264(1)	8542(1)	22(1)
C(32)	1820(1)	1830(1)	8769(1)	31(1)
C(33)	2698(1)	2004(1)	8692(1)	37(1)
C(34)	3141(1)	1632(1)	8383(1)	38(1)
C(35)	2709(1)	1076(2)	8155(1)	40(1)
C(36)	1831(1)	886(1)	8235(1)	32(1)
C(37)	281(1)	327(1)	9054(1)	23(1)
C(38)	1061(2)	-78(1)	9138(1)	33(1)
C(39)	1076(2)	-655(1)	9435(1)	42(1)
C(40)	320(2)	-838(1)	9644(1)	41(1)
C(41)	-459(2)	-444(1)	9562(1)	41(1)
C(42)	-480(2)	144(1)	9271(1)	31(1)
C(43)	-126(1)	456(1)	8221(1)	20(1)
C(44)	-305(1)	-348(1)	8245(1)	25(1)
C(45)	-561(1)	-762(1)	7902(1)	31(1)
C(46)	-611(1)	-387(1)	7535(1)	31(1)
C(47)	-430(1)	411(1)	7509(1)	30(1)
C(48)	-208(1)	832(1)	7851(1)	25(1)

Table 77. Bond lengths [Å] and angles [°] for Ru(IPr)(PPh_3)($CO)_3$ **(53)**.

Ru(1)-C(3)	1.9205(19)	C(19)-C(24)	1.402(3)
Ru(1)-C(1)	1.923(2)	C(19)-C(20)	1.403(3)
Ru(1)-C(2)	1.929(2)	C(20)-C(21)	1.392(3)
Ru(1)-C(4)	2.1268(17)	C(20)-C(25)	1.522(3)
Ru(1)-P(1)	2.3340(5)	C(21)-C(22)	1.383(3)
P(1)-C(37)	1.8301(19)	C(22)-C(23)	1.382(3)
P(1)-C(31)	1.8319(19)	C(23)-C(24)	1.398(3)
P(1)-C(43)	1.8331(19)	C(24)-C(28)	1.524(3)
O(1)-C(1)	1.159(2)	C(25)-C(26)	1.532(3)
O(2)-C(2)	1.158(2)	C(25)-C(27)	1.535(3)
O(3)-C(3)	1.152(2)	C(28)-C(29)	1.533(3)
N(1)-C(4)	1.374(2)	C(28)-C(30)	1.535(3)
N(1)-C(5)	1.392(2)	C(31)-C(36)	1.393(3)

N(1)-C(7)	1.447(2)	C(31)-C(32)	1.399(3)
N(2)-C(4)	1.374(2)	C(32)-C(33)	1.383(3)
N(2)-C(6)	1.392(2)	C(33)-C(34)	1.384(3)
N(2)-C(19)	1.441(2)	C(34)-C(35)	1.375(3)
C(5)-C(6)	1.339(3)	C(35)-C(36)	1.392(3)
C(7)-C(12)	1.398(3)	C(37)-C(42)	1.393(3)
C(7)-C(8)	1.406(3)	C(37)-C(38)	1.393(3)
C(8)-C(9)	1.399(3)	C(38)-C(39)	1.393(3)
C(8)-C(13)	1.516(3)	C(39)-C(40)	1.373(4)
C(9)-C(10)	1.377(3)	C(40)-C(41)	1.381(3)
C(10)-C(11)	1.381(3)	C(41)-C(42)	1.394(3)
C(11)-C(12)	1.398(3)	C(43)-C(44)	1.395(3)
C(12)-C(16)	1.520(3)	C(43)-C(48)	1.395(3)
C(13)-C(14)	1.533(3)	C(44)-C(45)	1.396(3)
C(13)-C(15)	1.541(3)	C(45)-C(46)	1.382(3)
C(16)-C(17)	1.529(3)	C(46)-C(47)	1.386(3)
C(16)-C(18)	1.536(3)	C(47)-C(48)	1.388(3)
C(3)-Ru(1)-C(1)	115.48(8)	C(12)-C(16)-C(17)	112.03(17)
C(3)-Ru(1)-C(2)	119.32(9)	C(12)-C(16)-C(18)	111.01(17)
C(1)-Ru(1)-C(2)	123.94(9)	C(17)-C(16)-C(18)	110.52(19)
C(3)-Ru(1)-C(4)	90.85(7)	C(24)-C(19)-C(20)	123.02(17)
C(1)-Ru(1)-C(4)	95.82(7)	C(24)-C(19)-N(2)	118.08(17)
C(2)-Ru(1)-C(4)	94.32(7)	C(20)-C(19)-N(2)	118.82(17)
C(3)-Ru(1)-P(1)	87.03(5)	C(21)-C(20)-C(19)	117.26(19)
C(1)-Ru(1)-P(1)	86.18(5)	C(21)-C(20)-C(25)	121.26(18)
C(2)-Ru(1)-P(1)	85.68(6)	C(19)-C(20)-C(25)	121.44(17)
C(4)-Ru(1)-P(1)	177.57(5)	C(22)-C(21)-C(20)	121.0(2)
C(37)-P(1)-C(31)	102.55(9)	C(23)-C(22)-C(21)	120.59(19)
C(37)-P(1)-C(43)	102.38(8)	C(22)-C(23)-C(24)	121.0(2)
C(31)-P(1)-C(43)	102.35(9)	C(23)-C(24)-C(19)	117.09(19)
C(37)-P(1)-Ru(1)	118.00(6)	C(23)-C(24)-C(28)	119.90(19)
C(31)-P(1)-Ru(1)	115.28(6)	C(19)-C(24)-C(28)	123.01(17)
C(43)-P(1)-Ru(1)	114.18(6)	C(20)-C(25)-C(26)	113.34(18)
C(4)-N(1)-C(5)	111.85(15)	C(20)-C(25)-C(27)	110.17(17)
C(4)-N(1)-C(7)	126.71(14)	C(26)-C(25)-C(27)	110.46(18)
C(5)-N(1)-C(7)	121.23(15)	C(24)-C(28)-C(29)	111.31(17)
C(4)-N(2)-C(6)	111.74(14)	C(24)-C(28)-C(30)	111.74(17)
C(4)-N(2)-C(19)	126.77(14)	C(29)-C(28)-C(30)	109.95(19)
C(6)-N(2)-C(19)	121.27(15)	C(36)-C(31)-C(32)	118.15(18)
O(1)-C(1)-Ru(1)	169.75(16)	C(36)-C(31)-P(1)	122.49(15)
O(2)-C(2)-Ru(1)	171.85(17)	C(32)-C(31)-P(1)	119.35(15)
O(3)-C(3)-Ru(1)	174.73(16)	C(33)-C(32)-C(31)	120.8(2)
N(2)-C(4)-N(1)	102.71(14)	C(32)-C(33)-C(34)	120.3(2)
N(2)-C(4)-Ru(1)	127.70(12)	C(35)-C(34)-C(33)	119.7(2)
N(1)-C(4)-Ru(1)	129.10(12)	C(34)-C(35)-C(36)	120.4(2)
C(6)-C(5)-N(1)	106.76(16)	C(35)-C(36)-C(31)	120.6(2)
C(5)-C(6)-N(2)	106.93(15)	C(42)-C(37)-C(38)	118.86(19)
C(12)-C(7)-C(8)	123.21(17)	C(42)-C(37)-P(1)	118.71(15)
C(12)-C(7)-N(1)	118.93(16)	C(38)-C(37)-P(1)	122.35(15)
C(8)-C(7)-N(1)	117.74(17)	C(39)-C(38)-C(37)	120.3(2)
C(9)-C(8)-C(7)	116.55(19)	C(40)-C(39)-C(38)	120.3(2)
C(9)-C(8)-C(13)	120.89(18)	C(39)-C(40)-C(41)	119.9(2)
C(7)-C(8)-C(13)	122.55(17)	C(40)-C(41)-C(42)	120.3(2)
C(10)-C(9)-C(8)	121.25(19)	C(37)-C(42)-C(41)	120.2(2)

C(9)-C(10)-C(11)	120.85(19)	C(44)-C(43)-C(48)	118.80(18)
C(10)-C(11)-C(12)	120.7(2)	C(44)-C(43)-P(1)	123.65(15)
C(7)-C(12)-C(11)	117.25(18)	C(48)-C(43)-P(1)	117.56(14)
C(7)-C(12)-C(16)	122.24(17)	C(43)-C(44)-C(45)	119.98(19)
C(11)-C(12)-C(16)	120.50(18)	C(46)-C(45)-C(44)	120.62(19)
C(8)-C(13)-C(14)	112.08(17)	C(45)-C(46)-C(47)	119.6(2)
C(8)-C(13)-C(15)	112.70(18)	C(46)-C(47)-C(48)	120.1(2)
C(14)-C(13)-C(15)	109.60(18)	C(47)-C(48)-C(43)	120.78(18)

Table 78. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(IPr)(PPh_3)($CO)_3$ **(53)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	18(1)	13(1)	19(1)	0(1)	1(1)	0(1)
P(1)	19(1)	15(1)	21(1)	1(1)	2(1)	1(1)
O(1)	47(1)	29(1)	26(1)	1(1)	-7(1)	8(1)
O(2)	30(1)	23(1)	77(1)	-10(1)	-6(1)	-3(1)
O(3)	35(1)	29(1)	30(1)	7(1)	8(1)	-2(1)
N(1)	19(1)	14(1)	21(1)	0(1)	-2(1)	-1(1)
N(2)	21(1)	16(1)	19(1)	0(1)	-3(1)	0(1)
C(1)	29(1)	17(1)	25(1)	0(1)	3(1)	4(1)
C(2)	24(1)	18(1)	41(1)	-2(1)	0(1)	4(1)
C(3)	26(1)	16(1)	25(1)	0(1)	0(1)	1(1)
C(4)	19(1)	15(1)	17(1)	1(1)	1(1)	-2(1)
C(5)	22(1)	15(1)	27(1)	2(1)	-2(1)	1(1)
C(6)	25(1)	13(1)	29(1)	-1(1)	-2(1)	2(1)
C(7)	21(1)	16(1)	23(1)	-1(1)	-5(1)	0(1)
C(8)	22(1)	19(1)	30(1)	0(1)	-1(1)	-1(1)
C(9)	25(1)	26(1)	41(1)	-2(1)	-3(1)	-8(1)
C(10)	37(1)	36(1)	36(1)	-10(1)	-9(1)	-12(1)
C(11)	34(1)	36(1)	25(1)	-6(1)	-4(1)	-3(1)
C(12)	23(1)	22(1)	24(1)	0(1)	-3(1)	0(1)
C(13)	29(1)	24(1)	35(1)	-3(1)	9(1)	-7(1)
C(14)	39(1)	46(1)	29(1)	3(1)	7(1)	-6(1)
C(15)	31(1)	36(1)	57(2)	-5(1)	15(1)	-3(1)
C(16)	25(1)	30(1)	24(1)	3(1)	-2(1)	-2(1)
C(17)	35(1)	51(1)	31(1)	-4(1)	8(1)	-5(1)
C(18)	40(1)	39(1)	52(2)	18(1)	2(1)	-2(1)
C(19)	27(1)	13(1)	22(1)	-3(1)	-7(1)	2(1)
C(20)	28(1)	15(1)	29(1)	-3(1)	-5(1)	1(1)
C(21)	30(1)	24(1)	40(1)	-2(1)	-12(1)	-2(1)
C(22)	44(1)	28(1)	35(1)	-3(1)	-21(1)	-1(1)
C(23)	47(1)	26(1)	23(1)	0(1)	-8(1)	3(1)
C(24)	36(1)	18(1)	22(1)	-2(1)	-4(1)	3(1)
C(25)	26(1)	23(1)	33(1)	-2(1)	-1(1)	-5(1)
C(26)	30(1)	45(1)	51(2)	-4(1)	4(1)	-4(1)
C(27)	50(1)	28(1)	37(1)	5(1)	5(1)	-2(1)
C(28)	36(1)	27(1)	22(1)	0(1)	-1(1)	1(1)
C(29)	44(1)	42(1)	40(1)	-7(1)	3(1)	7(1)
C(30)	48(2)	34(1)	42(2)	9(1)	8(1)	-1(1)
C(31)	20(1)	20(1)	26(1)	6(1)	-1(1)	3(1)
C(32)	26(1)	34(1)	33(1)	-3(1)	1(1)	4(1)
C(33)	26(1)	36(1)	48(2)	4(1)	-6(1)	-5(1)

C(34)	19(1)	45(1)	48(2)	16(1)	1(1)	0(1)
C(35)	25(1)	55(2)	41(1)	0(1)	7(1)	8(1)
C(36)	26(1)	34(1)	36(1)	-3(1)	4(1)	3(1)
C(37)	31(1)	16(1)	22(1)	-1(1)	1(1)	-1(1)
C(38)	34(1)	26(1)	39(1)	10(1)	-5(1)	0(1)
C(39)	50(2)	31(1)	45(2)	11(1)	-14(1)	4(1)
C(40)	71(2)	23(1)	30(1)	7(1)	-4(1)	-2(1)
C(41)	61(2)	30(1)	31(1)	6(1)	16(1)	-3(1)
C(42)	40(1)	25(1)	29(1)	3(1)	9(1)	1(1)
C(43)	19(1)	19(1)	23(1)	-2(1)	2(1)	3(1)
C(44)	25(1)	21(1)	30(1)	-3(1)	5(1)	-2(1)
C(45)	28(1)	26(1)	40(1)	-11(1)	8(1)	-5(1)
C(46)	24(1)	37(1)	33(1)	-14(1)	2(1)	-3(1)
C(47)	27(1)	37(1)	25(1)	-3(1)	-1(1)	4(1)
C(48)	27(1)	22(1)	26(1)	1(1)	2(1)	2(1)

Table 79. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(IPr)(PPh_3)($CO)_3$ **(53)**.

Atom	x	y	z	U(eq)
H(5)	-2954	4459	8598	26
H(6)	-1933	4929	9125	27
H(9)	-4455	1806	8312	37
H(10)	-4015	1681	7652	43
H(11)	-2822	2391	7406	38
H(13)	-3604	3198	9009	35
H(14A)	-3525	1530	9122	57
H(14B)	-3552	2163	9477	57
H(14C)	-2710	2119	9187	57
H(15A)	-5081	2975	8769	62
H(15B)	-4974	2761	9234	62
H(15C)	-5000	2075	8906	62
H(16)	-1273	3470	8001	31
H(17A)	-1531	2900	7204	59
H(17B)	-1070	2378	7545	59
H(17C)	-615	3179	7399	59
H(18A)	-2406	4091	7389	65
H(18B)	-1478	4469	7517	65
H(18C)	-2288	4466	7826	65
H(21)	1366	4400	9552	37
H(22)	953	4109	10206	43
H(23)	-467	3670	10349	38
H(25)	45	4083	8678	33
H(26A)	1791	4528	8919	63
H(26B)	1494	4299	8473	63
H(26C)	1514	3641	8817	63
H(27A)	-377	5376	8864	58
H(27B)	353	5399	8516	58
H(27C)	630	5580	8970	58
H(28)	-2212	3382	9622	34
H(29A)	-2954	3827	10198	63
H(29B)	-2348	4524	10029	63
H(29C)	-2033	4030	10411	63
H(30A)	-1511	2613	10318	62

H(30B)	-1594	2219	9884	62
H(30C)	-2467	2436	10132	62
H(32)	1518	2099	8978	37
H(33)	2999	2380	8853	44
H(34)	3740	1759	8327	45
H(35)	3012	821	7942	48
H(36)	1542	495	8079	38
H(38)	1585	39	8993	40
H(39)	1612	-924	9493	50
H(40)	332	-1234	9844	49
H(41)	-982	-574	9704	49
H(42)	-1014	421	9220	38
H(44)	-253	-615	8494	30
H(45)	-703	-1305	7921	37
H(46)	-768	-675	7301	38
H(47)	-458	670	7257	36
H(48)	-111	1384	7833	30

Table 80. Crystal data and structure refinement for $Ru(SIPr)(PPh_3)(CO)_3$ **(54)**.

Compound	$Ru(SIPr)(PPh_3)(CO)_3$ **(54)**
Empirical formula	C48 H53 N2 O3 P Ru
Formula weight	837.96
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 15.04700(10)Å α = 90°
	b = 17.00600(10)Å β = 90°
	c = 33.5150(2)Å γ = 90°
Volume	8576.13(9) $Å^3$
Z	8
Density (calculated)	1.298 Mg/m^3
Absorption coefficient	0.445 mm^{-1}
F(000)	3504
Crystal size	0.50 x 0.50 x 0.35 mm
Theta range for data collection	3.54 to 30.01°
Index ranges	-21<=h<=21; -23<=k<=23; -47<=l<=47
Reflections collected	123510
Independent reflections	12471 [R(int) = 0.0523]
Reflections observed (>2σ)	9995
Data Completeness	0.997
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.86 and 0.81
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12471 / 0 / 504
Goodness-of-fit on F^2	1.040
Final R indices [I>2σ(I)]	R1 = 0.0295 wR2 = 0.0667
R indices (all data)	R1 = 0.0443 wR2 = 0.0725
Largest diff. peak and hole	0.673 and -0.733 $eÅ^{-3}$

Table 81. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ru(SIPr)(PPh_3)(CO)_3$ **(54)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	-700(1)	2184(1)	6242(1)	16(1)
P(1)	200(1)	1079(1)	6344(1)	18(1)
O(3)	449(1)	2976(1)	6883(1)	32(1)
O(2)	190(1)	2118(1)	5419(1)	32(1)
O(1)	-2174(1)	1047(1)	6511(1)	40(1)
N(1)	-1308(1)	3833(1)	5937(1)	20(1)
N(2)	-2223(1)	3409(1)	6387(1)	19(1)
C(1)	-1671(1)	1517(1)	6408(1)	26(1)
C(2)	-200(1)	2198(1)	5713(1)	23(1)
C(3)	-10(1)	2707(1)	6644(1)	22(1)
C(4)	-1493(1)	3204(1)	6173(1)	17(1)
C(5)	-1969(1)	4472(1)	5966(1)	24(1)
C(6)	-2474(1)	4245(1)	6340(1)	23(1)
C(7)	-663(1)	3875(1)	5620(1)	21(1)
C(8)	-927(1)	3680(1)	5231(1)	24(1)
C(9)	-302(1)	3780(1)	4926(1)	32(1)
C(10)	541(1)	4059(1)	5005(1)	35(1)
C(11)	786(1)	4244(1)	5391(1)	32(1)
C(12)	192(1)	4162(1)	5708(1)	24(1)
C(13)	-1852(1)	3375(1)	5129(1)	28(1)
C(14)	-2345(1)	3945(1)	4850(1)	39(1)
C(15)	-1823(1)	2553(1)	4940(1)	38(1)
C(16)	454(1)	4406(1)	6127(1)	28(1)
C(17)	324(2)	5294(1)	6184(1)	43(1)
C(18)	1407(1)	4176(1)	6236(1)	43(1)
C(19)	-2736(1)	2932(1)	6656(1)	20(1)
C(20)	-2512(1)	2904(1)	7062(1)	23(1)
C(21)	-3039(1)	2439(1)	7312(1)	32(1)
C(22)	-3754(1)	2025(1)	7162(1)	36(1)
C(23)	-3987(1)	2087(1)	6765(1)	30(1)
C(24)	-3497(1)	2557(1)	6502(1)	24(1)
C(25)	-1738(1)	3364(1)	7236(1)	26(1)
C(26)	-1185(1)	2852(1)	7519(1)	37(1)
C(27)	-2058(1)	4103(1)	7458(1)	39(1)
C(28)	-3787(1)	2657(1)	6070(1)	28(1)
C(29)	-4802(1)	2625(1)	6020(1)	40(1)
C(30)	-3352(1)	2053(1)	5794(1)	36(1)
C(31)	-113(1)	465(1)	6771(1)	21(1)
C(32)	-206(1)	833(1)	7142(1)	26(1)
C(33)	-414(1)	402(1)	7481(1)	31(1)
C(34)	-568(1)	-402(1)	7450(1)	33(1)
C(35)	-502(1)	-768(1)	7084(1)	33(1)
C(36)	-261(1)	-343(1)	6746(1)	26(1)
C(37)	1371(1)	1294(1)	6449(1)	22(1)
C(38)	1837(1)	931(1)	6758(1)	34(1)
C(39)	2716(1)	1133(1)	6834(1)	42(1)
C(40)	3143(1)	1681(1)	6601(1)	38(1)
C(41)	2695(1)	2037(1)	6290(1)	38(1)
C(42)	1812(1)	1851(1)	6216(1)	32(1)

C(43)	268(1)	357(1)	5940(1)	22(1)
C(44)	1049(1)	-53(1)	5855(1)	32(1)
C(45)	1057(1)	-631(1)	5559(1)	38(1)
C(46)	293(1)	-812(1)	5354(1)	37(1)
C(47)	-487(1)	-410(1)	5437(1)	35(1)
C(48)	-501(1)	178(1)	5727(1)	28(1)

Table 82. Bond lengths [Å] and angles [°] for Ru(SIPr)(PPh_3)($CO)_3$ **(54)**.

Ru(1)-C(3)	1.9174(15)	C(19)-C(20)	1.401(2)
Ru(1)-C(2)	1.9267(15)	C(19)-C(24)	1.408(2)
Ru(1)-C(1)	1.9315(16)	C(20)-C(21)	1.398(2)
Ru(1)-C(4)	2.1193(14)	C(20)-C(25)	1.521(2)
Ru(1)-P(1)	2.3409(4)	C(21)-C(22)	1.380(3)
P(1)-C(43)	1.8311(15)	C(22)-C(23)	1.382(2)
P(1)-C(31)	1.8318(15)	C(23)-C(24)	1.398(2)
P(1)-C(37)	1.8343(15)	C(24)-C(28)	1.522(2)
O(3)-C(3)	1.1535(18)	C(25)-C(26)	1.532(2)
O(2)-C(2)	1.1545(18)	C(25)-C(27)	1.539(2)
O(1)-C(1)	1.1531(19)	C(28)-C(30)	1.530(2)
N(1)-C(4)	1.3602(17)	C(28)-C(29)	1.537(2)
N(1)-C(7)	1.4383(18)	C(31)-C(36)	1.394(2)
N(1)-C(5)	1.4767(18)	C(31)-C(32)	1.398(2)
N(2)-C(4)	1.3561(17)	C(32)-C(33)	1.389(2)
N(2)-C(19)	1.4384(17)	C(33)-C(34)	1.391(2)
N(2)-C(6)	1.4789(18)	C(34)-C(35)	1.378(3)
C(5)-C(6)	1.515(2)	C(35)-C(36)	1.392(2)
C(7)-C(8)	1.405(2)	C(37)-C(38)	1.393(2)
C(7)-C(12)	1.407(2)	C(37)-C(42)	1.395(2)
C(8)-C(9)	1.400(2)	C(38)-C(39)	1.391(2)
C(8)-C(13)	1.524(2)	C(39)-C(40)	1.376(3)
C(9)-C(10)	1.380(3)	C(40)-C(41)	1.379(3)
C(10)-C(11)	1.384(3)	C(41)-C(42)	1.389(2)
C(11)-C(12)	1.394(2)	C(43)-C(48)	1.394(2)
C(12)-C(16)	1.518(2)	C(43)-C(44)	1.396(2)
C(13)-C(15)	1.534(2)	C(44)-C(45)	1.395(2)
C(13)-C(14)	1.536(2)	C(45)-C(46)	1.375(3)
C(16)-C(18)	1.532(2)	C(46)-C(47)	1.386(3)
C(16)-C(17)	1.534(2)	C(47)-C(48)	1.394(2)
C(3)-Ru(1)-C(2)	115.35(6)	C(12)-C(16)-C(18)	113.22(15)
C(3)-Ru(1)-C(1)	118.72(7)	C(12)-C(16)-C(17)	110.66(14)
C(2)-Ru(1)-C(1)	124.58(7)	C(18)-C(16)-C(17)	109.91(15)
C(3)-Ru(1)-C(4)	90.11(5)	C(20)-C(19)-C(24)	122.32(13)
C(2)-Ru(1)-C(4)	96.25(5)	C(20)-C(19)-N(2)	119.92(13)
C(1)-Ru(1)-C(4)	94.92(6)	C(24)-C(19)-N(2)	117.55(13)
C(3)-Ru(1)-P(1)	87.55(4)	C(21)-C(20)-C(19)	117.65(14)
C(2)-Ru(1)-P(1)	85.33(4)	C(21)-C(20)-C(25)	119.63(14)
C(1)-Ru(1)-P(1)	85.65(4)	C(19)-C(20)-C(25)	122.72(13)
C(4)-Ru(1)-P(1)	177.58(4)	C(22)-C(21)-C(20)	120.88(15)
C(43)-P(1)-C(31)	102.15(7)	C(21)-C(22)-C(23)	120.59(15)
C(43)-P(1)-C(37)	102.76(7)	C(22)-C(23)-C(24)	121.06(16)
C(31)-P(1)-C(37)	102.20(7)	C(23)-C(24)-C(19)	117.24(14)
C(43)-P(1)-Ru(1)	117.55(5)	C(23)-C(24)-C(28)	120.71(14)
C(31)-P(1)-Ru(1)	115.00(5)	C(19)-C(24)-C(28)	122.04(13)

C(37)-P(1)-Ru(1)	115.06(5)	C(20)-C(25)-C(26)	111.29(13)
C(4)-N(1)-C(7)	127.34(12)	C(20)-C(25)-C(27)	111.49(13)
C(4)-N(1)-C(5)	113.66(11)	C(26)-C(25)-C(27)	109.60(14)
C(7)-N(1)-C(5)	117.85(11)	C(24)-C(28)-C(30)	112.26(13)
C(4)-N(2)-C(19)	128.31(11)	C(24)-C(28)-C(29)	112.61(14)
C(4)-N(2)-C(6)	113.44(11)	C(30)-C(28)-C(29)	109.60(14)
C(19)-N(2)-C(6)	118.19(11)	C(36)-C(31)-C(32)	118.59(14)
O(1)-C(1)-Ru(1)	171.62(13)	C(36)-C(31)-P(1)	123.75(12)
O(2)-C(2)-Ru(1)	169.19(13)	C(32)-C(31)-P(1)	117.65(11)
O(3)-C(3)-Ru(1)	174.95(13)	C(33)-C(32)-C(31)	120.86(15)
N(2)-C(4)-N(1)	105.77(11)	C(32)-C(33)-C(34)	119.76(16)
N(2)-C(4)-Ru(1)	127.51(9)	C(35)-C(34)-C(33)	119.82(16)
N(1)-C(4)-Ru(1)	126.29(10)	C(34)-C(35)-C(36)	120.58(16)
N(1)-C(5)-C(6)	101.85(11)	C(35)-C(36)-C(31)	120.31(15)
N(2)-C(6)-C(5)	101.81(11)	C(38)-C(37)-C(42)	118.48(15)
C(8)-C(7)-C(12)	122.26(13)	C(38)-C(37)-P(1)	122.49(12)
C(8)-C(7)-N(1)	118.87(13)	C(42)-C(37)-P(1)	119.02(12)
C(12)-C(7)-N(1)	118.72(13)	C(39)-C(38)-C(37)	120.43(17)
C(9)-C(8)-C(7)	117.41(15)	C(40)-C(39)-C(38)	120.38(17)
C(9)-C(8)-C(13)	119.38(14)	C(39)-C(40)-C(41)	119.88(16)
C(7)-C(8)-C(13)	123.20(13)	C(40)-C(41)-C(42)	120.19(18)
C(10)-C(9)-C(8)	121.26(16)	C(41)-C(42)-C(37)	120.62(16)
C(9)-C(10)-C(11)	120.23(15)	C(48)-C(43)-C(44)	119.03(14)
C(10)-C(11)-C(12)	121.22(16)	C(48)-C(43)-P(1)	118.63(12)
C(11)-C(12)-C(7)	117.62(15)	C(44)-C(43)-P(1)	122.22(12)
C(11)-C(12)-C(16)	120.69(15)	C(45)-C(44)-C(43)	120.26(16)
C(7)-C(12)-C(16)	121.65(13)	C(46)-C(45)-C(44)	120.37(17)
C(8)-C(13)-C(15)	112.14(14)	C(45)-C(46)-C(47)	119.86(15)
C(8)-C(13)-C(14)	111.22(14)	C(46)-C(47)-C(48)	120.38(17)
C(15)-C(13)-C(14)	109.79(14)	C(43)-C(48)-C(47)	120.08(16)

Table 83. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(SIPr)(PPh_3)(CO)_3$ **(54)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	17(1)	13(1)	18(1)	0(1)	-1(1)	0(1)
P(1)	18(1)	15(1)	21(1)	-1(1)	-2(1)	1(1)
O(3)	34(1)	32(1)	30(1)	-7(1)	-7(1)	-3(1)
O(2)	42(1)	30(1)	24(1)	-1(1)	6(1)	8(1)
O(1)	28(1)	22(1)	71(1)	10(1)	6(1)	-2(1)
N(1)	22(1)	16(1)	22(1)	1(1)	5(1)	2(1)
N(2)	20(1)	14(1)	22(1)	1(1)	4(1)	-1(1)
C(1)	22(1)	19(1)	36(1)	2(1)	-1(1)	4(1)
C(2)	26(1)	18(1)	23(1)	0(1)	-1(1)	4(1)
C(3)	24(1)	17(1)	26(1)	0(1)	0(1)	2(1)
C(4)	18(1)	15(1)	17(1)	-2(1)	-1(1)	-3(1)
C(5)	26(1)	18(1)	29(1)	3(1)	6(1)	4(1)
C(6)	25(1)	16(1)	28(1)	2(1)	6(1)	3(1)
C(7)	24(1)	15(1)	24(1)	3(1)	7(1)	2(1)
C(8)	32(1)	18(1)	23(1)	2(1)	5(1)	3(1)
C(9)	46(1)	26(1)	24(1)	1(1)	11(1)	4(1)
C(10)	42(1)	29(1)	34(1)	2(1)	20(1)	1(1)
C(11)	29(1)	25(1)	41(1)	2(1)	12(1)	-3(1)

C(12)	26(1)	16(1)	30(1)	2(1)	6(1)	0(1)
C(13)	33(1)	27(1)	23(1)	-1(1)	2(1)	2(1)
C(14)	42(1)	42(1)	32(1)	4(1)	-1(1)	9(1)
C(15)	44(1)	34(1)	37(1)	-10(1)	-5(1)	1(1)
C(16)	27(1)	23(1)	34(1)	2(1)	2(1)	-5(1)
C(17)	56(1)	29(1)	44(1)	-8(1)	-8(1)	-1(1)
C(18)	29(1)	46(1)	53(1)	4(1)	-6(1)	-3(1)
C(19)	20(1)	16(1)	23(1)	1(1)	5(1)	0(1)
C(20)	22(1)	23(1)	24(1)	0(1)	3(1)	1(1)
C(21)	33(1)	37(1)	25(1)	6(1)	6(1)	-2(1)
C(22)	34(1)	36(1)	37(1)	10(1)	11(1)	-9(1)
C(23)	25(1)	27(1)	40(1)	2(1)	3(1)	-7(1)
C(24)	22(1)	20(1)	29(1)	1(1)	2(1)	0(1)
C(25)	25(1)	28(1)	23(1)	-2(1)	1(1)	-2(1)
C(26)	34(1)	45(1)	32(1)	5(1)	-6(1)	-1(1)
C(27)	37(1)	39(1)	41(1)	-14(1)	-1(1)	1(1)
C(28)	28(1)	24(1)	33(1)	4(1)	-6(1)	-7(1)
C(29)	30(1)	33(1)	56(1)	4(1)	-14(1)	-2(1)
C(30)	35(1)	43(1)	29(1)	-4(1)	-5(1)	-5(1)
C(31)	18(1)	21(1)	24(1)	2(1)	-3(1)	1(1)
C(32)	29(1)	23(1)	26(1)	1(1)	0(1)	3(1)
C(33)	29(1)	37(1)	27(1)	5(1)	1(1)	3(1)
C(34)	26(1)	40(1)	34(1)	15(1)	-2(1)	-4(1)
C(35)	32(1)	26(1)	42(1)	10(1)	-10(1)	-7(1)
C(36)	26(1)	22(1)	30(1)	2(1)	-8(1)	-2(1)
C(37)	18(1)	23(1)	26(1)	-5(1)	-1(1)	3(1)
C(38)	25(1)	41(1)	35(1)	4(1)	-4(1)	3(1)
C(39)	24(1)	61(1)	41(1)	-1(1)	-10(1)	7(1)
C(40)	17(1)	51(1)	47(1)	-18(1)	-1(1)	1(1)
C(41)	26(1)	41(1)	48(1)	-5(1)	5(1)	-5(1)
C(42)	24(1)	34(1)	37(1)	2(1)	-1(1)	0(1)
C(43)	28(1)	17(1)	22(1)	-1(1)	0(1)	0(1)
C(44)	30(1)	28(1)	37(1)	-9(1)	3(1)	2(1)
C(45)	44(1)	29(1)	41(1)	-11(1)	9(1)	6(1)
C(46)	59(1)	24(1)	27(1)	-8(1)	4(1)	-4(1)
C(47)	48(1)	29(1)	26(1)	-5(1)	-7(1)	-5(1)
C(48)	33(1)	24(1)	27(1)	-3(1)	-5(1)	0(1)

Table 84. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Ru(SIPr)(PPh_3)($CO)_3$ **(54)**.

Atom	x	y	z	U(eq)
H(5A)	-2364	4482	5730	29
H(5B)	-1679	4991	5996	29
H(6A)	-2282	4562	6572	28
H(6B)	-3123	4305	6303	28
H(9)	-461	3654	4659	38
H(10)	954	4124	4793	42
H(11)	1371	4429	5442	38
H(13)	-2198	3336	5382	33
H(14A)	-2362	4468	4972	58
H(14B)	-2953	3757	4808	58
H(14C)	-2034	3974	4594	58
H(15A)	-1469	2571	4694	57

H(15B)	-2429	2382	4876	57
H(15C)	-1553	2182	5128	57
H(16)	46	4131	6317	33
H(17A)	751	5579	6018	64
H(17B)	421	5429	6465	64
H(17C)	-282	5439	6107	64
H(18A)	1493	3613	6187	64
H(18B)	1513	4289	6519	64
H(18C)	1825	4478	6073	64
H(21)	-2904	2409	7588	38
H(22)	-4089	1694	7334	43
H(23)	-4488	1806	6668	37
H(25)	-1346	3535	7012	31
H(26A)	-1508	2779	7770	55
H(26B)	-615	3112	7573	55
H(26C)	-1076	2339	7395	55
H(27A)	-2409	4431	7276	59
H(27B)	-1543	4402	7553	59
H(27C)	-2427	3948	7686	59
H(28)	-3587	3189	5981	34
H(29A)	-5012	2090	6074	60
H(29B)	-4959	2774	5747	60
H(29C)	-5081	2991	6208	60
H(30A)	-2704	2108	5807	53
H(30B)	-3551	2143	5519	53
H(30C)	-3522	1522	5878	53
H(32)	-125	1386	7162	31
H(33)	-451	655	7733	37
H(34)	-718	-699	7681	40
H(35)	-623	-1314	7062	40
H(36)	-198	-604	6497	31
H(38)	1552	544	6917	40
H(39)	3025	891	7049	51
H(40)	3744	1815	6653	46
H(41)	2992	2409	6126	46
H(42)	1504	2105	6005	38
H(44)	1577	62	5999	38
H(45)	1594	-900	5499	46
H(46)	299	-1211	5156	44
H(47)	-1015	-536	5295	41
H(48)	-1036	456	5779	34

Table 85. Crystal data and structure refinement for Ru(dppp)(PPh_3)(CO)HF **(62)**.

Compound	Ru(dppp)(PPh_3)(CO)HF **(62)**
Empirical formula	C46 H42 F O P3 Ru
Formula weight	823.78
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.1880(2)Å α = 95.101(1)^o
	b = 16.7830(3)Å β = 92.783(1)^o
	c = 23.0560(5)Å γ = 90.684(1)^o
Volume	3921.47(13) Å^3
Z	4
Density (calculated)	1.395 Mg/m^3
Absorption coefficient	0.562 mm^{-1}
F(000)	1696
Crystal size	0.15 x 0.15 x 0.12 mm
Theta range for data collection	3.53 to 27.49^o
Index ranges	-13<=h<=13; -21<=k<=21; -29<=l<=29
Reflections collected	71302
Independent reflections	17384 [R(int) = 0.0705]
Reflections observed (>2σ)	11929
Data Completeness	0.965
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.94 and 0.88
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17384 / 2 / 939
Goodness-of-fit on F^2	1.057
Final R indices [I>2σ(I)]	R^1 = 0.0473 wR_2 = 0.0836
R indices (all data)	R^1 = 0.0878 wR_2 = 0.0972
Largest diff. peak and hole	0.515 and -0.506 eÅ^{-3}

Table 86. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Ru(dppp)(PPh_3)(CO)HF **(62)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	1207(1)	-1166(1)	2314(1)	23(1)
Ru(2)	-2411(1)	-6132(1)	2454(1)	23(1)
P(1)	1624(1)	-313(1)	3176(1)	25(1)
P(2)	-1127(1)	-1427(1)	2408(1)	25(1)
P(3)	1269(1)	-2025(1)	1460(1)	25(1)
P(4)	-2592(1)	-5336(1)	3351(1)	24(1)
P(5)	-2582(1)	-6891(1)	1551(1)	26(1)
P(6)	-65(1)	-6393(1)	2561(1)	24(1)
F(1)	1329(2)	-2252(1)	2701(1)	28(1)
F(2)	-2521(2)	-7262(1)	2770(1)	29(1)
O(1)	1266(3)	313(2)	1686(1)	37(1)
O(2)	-2586(3)	-4584(2)	1919(1)	39(1)
C(1)	1208(3)	-265(2)	1932(2)	27(1)
C(2)	2812(3)	499(2)	3089(2)	28(1)
C(3)	2626(4)	1291(2)	3290(2)	33(1)

C(4)	3635(4)	1855(2)	3276(2)	41(1)
C(5)	4837(4)	1627(2)	3065(2)	41(1)
C(6)	5016(4)	844(2)	2855(2)	40(1)
C(7)	4020(4)	289(2)	2867(2)	34(1)
C(8)	2438(3)	-713(2)	3814(2)	28(1)
C(9)	2953(4)	-189(2)	4278(2)	34(1)
C(10)	3573(4)	-486(2)	4758(2)	36(1)
C(11)	3723(4)	-1299(2)	4774(2)	39(1)
C(12)	3227(4)	-1816(2)	4315(2)	41(1)
C(13)	2576(4)	-1526(2)	3835(2)	35(1)
C(14)	237(3)	238(2)	3474(2)	28(1)
C(15)	-86(4)	264(2)	4053(2)	34(1)
C(16)	-1116(4)	733(2)	4254(2)	43(1)
C(17)	-1823(4)	1177(2)	3877(2)	42(1)
C(18)	-1530(4)	1152(2)	3301(2)	34(1)
C(19)	-505(3)	686(2)	3097(2)	30(1)
C(20)	-1502(4)	-2496(2)	2195(2)	31(1)
C(21)	-1294(4)	-2758(2)	1556(2)	33(1)
C(22)	158(3)	-2897(2)	1426(2)	32(1)
C(23)	-2411(3)	-942(2)	1983(2)	28(1)
C(24)	-3694(4)	-1236(2)	1928(2)	36(1)
C(25)	-4648(4)	-881(2)	1593(2)	42(1)
C(26)	-4334(4)	-227(2)	1306(2)	41(1)
C(27)	-3066(4)	78(2)	1354(2)	43(1)
C(28)	-2107(4)	-278(2)	1688(2)	36(1)
C(29)	-1729(3)	-1370(2)	3150(2)	29(1)
C(30)	-2826(4)	-954(2)	3326(2)	35(1)
C(31)	-3267(4)	-976(2)	3881(2)	42(1)
C(32)	-2592(4)	-1407(3)	4273(2)	46(1)
C(33)	-1475(5)	-1821(2)	4110(2)	47(1)
C(34)	-1044(4)	-1803(2)	3556(2)	36(1)
C(35)	978(4)	-1585(2)	768(2)	31(1)
C(36)	1846(4)	-997(2)	627(2)	38(1)
C(37)	1666(5)	-644(3)	107(2)	48(1)
C(38)	617(5)	-866(3)	-271(2)	53(1)
C(39)	-251(5)	-1450(3)	-140(2)	51(1)
C(40)	-80(4)	-1819(3)	378(2)	41(1)
C(41)	2824(3)	-2545(2)	1350(2)	26(1)
C(42)	3268(4)	-2761(2)	798(2)	36(1)
C(43)	4426(4)	-3181(2)	729(2)	39(1)
C(44)	5137(4)	-3404(2)	1211(2)	34(1)
C(45)	4696(4)	-3209(2)	1761(2)	33(1)
C(46)	3552(4)	-2777(2)	1833(2)	32(1)
C(47)	-2478(3)	-5187(2)	2124(2)	28(1)
C(48)	-3190(3)	-5803(2)	3978(2)	26(1)
C(49)	-3387(4)	-5379(2)	4517(2)	35(1)
C(50)	-3951(4)	-5748(2)	4961(2)	37(1)
C(51)	-4375(4)	-6533(2)	4872(2)	37(1)
C(52)	-4208(4)	-6958(2)	4340(2)	43(1)
C(53)	-3607(4)	-6603(2)	3897(2)	37(1)
C(54)	-3825(3)	-4546(2)	3305(2)	26(1)
C(55)	-3577(4)	-3748(2)	3501(2)	33(1)
C(56)	-4571(4)	-3184(2)	3468(2)	37(1)
C(57)	-5804(4)	-3409(2)	3249(2)	34(1)
C(58)	-6071(4)	-4200(2)	3052(2)	36(1)

C(59)	-5081(3)	-4761(2)	3083(2)	32(1)
C(60)	-1119(3)	-4753(2)	3614(1)	26(1)
C(61)	-516(4)	-4769(2)	4165(2)	37(1)
C(62)	595(4)	-4308(3)	4328(2)	46(1)
C(63)	1116(4)	-3813(2)	3950(2)	39(1)
C(64)	548(4)	-3796(2)	3397(2)	33(1)
C(65)	-551(3)	-4267(2)	3230(2)	30(1)
C(66)	-1486(4)	-7750(2)	1464(2)	31(1)
C(67)	-23(3)	-7646(2)	1652(2)	32(1)
C(68)	235(3)	-7441(2)	2306(2)	27(1)
C(69)	-4124(4)	-7438(2)	1337(2)	30(1)
C(70)	-4950(4)	-7644(2)	1758(2)	36(1)
C(71)	-6056(4)	-8139(2)	1605(2)	43(1)
C(72)	-6328(4)	-8414(2)	1034(2)	46(1)
C(73)	-5507(5)	-8215(3)	608(2)	53(1)
C(74)	-4412(4)	-7731(3)	757(2)	44(1)
C(75)	-2356(4)	-6307(2)	930(2)	31(1)
C(76)	-3308(4)	-5741(2)	809(2)	38(1)
C(77)	-3149(5)	-5235(2)	373(2)	46(1)
C(78)	-2038(5)	-5279(3)	56(2)	50(1)
C(79)	-1106(5)	-5837(3)	164(2)	49(1)
C(80)	-1259(4)	-6354(2)	597(2)	38(1)
C(81)	661(3)	-6403(2)	3303(2)	27(1)
C(82)	19(4)	-6864(2)	3677(2)	37(1)
C(83)	536(5)	-6942(3)	4235(2)	47(1)
C(84)	1698(4)	-6562(3)	4431(2)	47(1)
C(85)	2343(4)	-6093(3)	4067(2)	47(1)
C(86)	1821(4)	-6005(2)	3509(2)	36(1)
C(87)	1157(3)	-5883(2)	2161(2)	27(1)
C(88)	802(4)	-5237(2)	1851(2)	36(1)
C(89)	1700(4)	-4881(2)	1518(2)	41(1)
C(90)	2958(4)	-5159(2)	1486(2)	37(1)
C(91)	3326(4)	-5797(2)	1790(2)	39(1)
C(92)	2432(3)	-6157(2)	2122(2)	37(1)

Table 87. Bond lengths [Å] and angles [°] for Ru(dppp)(PPh_3)(CO)HF **(62)**.

Ru(1)-H(1)	1.4944	Ru(1)-C(1)	1.816(4)
Ru(1)-F(1)	2.1005(18)	Ru(1)-P(3)	2.3390(9)
Ru(1)-P(1)	2.3622(9)	Ru(1)-P(2)	2.4354(9)
Ru(2)-H(2)	1.4657	Ru(2)-C(47)	1.820(4)
Ru(2)-F(2)	2.0943(18)	Ru(2)-P(5)	2.3418(9)
Ru(2)-P(4)	2.3752(9)	Ru(2)-P(6)	2.4396(9)
P(1)-C(14)	1.826(3)	P(1)-C(8)	1.836(3)
P(1)-C(2)	1.841(4)	P(2)-C(23)	1.838(3)
P(2)-C(29)	1.841(4)	P(2)-C(20)	1.848(4)
P(3)-C(35)	1.830(4)	P(3)-C(22)	1.833(4)
P(3)-C(41)	1.835(3)	P(4)-C(60)	1.830(4)
P(4)-C(48)	1.830(4)	P(4)-C(54)	1.843(3)
P(5)-C(75)	1.828(4)	P(5)-C(69)	1.834(4)
P(5)-C(66)	1.836(3)	P(6)-C(81)	1.834(3)
P(6)-C(87)	1.833(4)	P(6)-C(68)	1.839(3)
O(1)-C(1)	1.169(4)	O(2)-C(47)	1.158(4)
C(2)-C(3)	1.387(5)	C(2)-C(7)	1.393(5)
C(3)-C(4)	1.392(5)	C(4)-C(5)	1.385(6)

C(5)-C(6)	1.377(5)	C(6)-C(7)	1.371(5)
C(8)-C(13)	1.378(5)	C(8)-C(9)	1.401(5)
C(9)-C(10)	1.381(5)	C(10)-C(11)	1.378(5)
C(11)-C(12)	1.378(5)	C(12)-C(13)	1.391(5)
C(14)-C(15)	1.387(5)	C(14)-C(19)	1.400(5)
C(15)-C(16)	1.392(5)	C(16)-C(17)	1.377(6)
C(17)-C(18)	1.374(5)	C(18)-C(19)	1.387(5)
C(20)-C(21)	1.526(5)	C(21)-C(22)	1.539(5)
C(23)-C(24)	1.387(5)	C(23)-C(28)	1.395(5)
C(24)-C(25)	1.386(5)	C(25)-C(26)	1.373(6)
C(26)-C(27)	1.380(6)	C(27)-C(28)	1.389(5)
C(29)-C(30)	1.384(5)	C(29)-C(34)	1.399(5)
C(30)-C(31)	1.380(5)	C(31)-C(32)	1.372(6)
C(32)-C(33)	1.390(6)	C(33)-C(34)	1.374(5)
C(35)-C(36)	1.389(5)	C(35)-C(40)	1.399(5)
C(36)-C(37)	1.388(5)	C(37)-C(38)	1.373(6)
C(38)-C(39)	1.376(7)	C(39)-C(40)	1.396(6)
C(41)-C(42)	1.391(5)	C(41)-C(46)	1.395(5)
C(42)-C(43)	1.390(5)	C(43)-C(44)	1.378(5)
C(44)-C(45)	1.380(5)	C(45)-C(46)	1.388(5)
C(48)-C(53)	1.397(5)	C(48)-C(49)	1.400(5)
C(49)-C(50)	1.387(5)	C(50)-C(51)	1.376(5)
C(51)-C(52)	1.383(5)	C(52)-C(53)	1.390(5)
C(54)-C(59)	1.387(5)	C(54)-C(55)	1.392(5)
C(55)-C(56)	1.398(5)	C(56)-C(57)	1.368(5)
C(57)-C(58)	1.383(5)	C(58)-C(59)	1.392(5)
C(60)-C(61)	1.387(5)	C(60)-C(65)	1.397(5)
C(61)-C(62)	1.382(5)	C(62)-C(63)	1.378(6)
C(63)-C(64)	1.377(5)	C(64)-C(65)	1.382(5)
C(66)-C(67)	1.535(5)	C(67)-C(68)	1.526(5)
C(69)-C(70)	1.380(5)	C(69)-C(74)	1.398(5)
C(70)-C(71)	1.404(5)	C(71)-C(72)	1.371(6)
C(72)-C(73)	1.380(6)	C(73)-C(74)	1.383(6)
C(75)-C(80)	1.385(5)	C(75)-C(76)	1.402(5)
C(76)-C(77)	1.386(5)	C(77)-C(78)	1.376(6)
C(78)-C(79)	1.371(6)	C(79)-C(80)	1.393(6)
C(81)-C(82)	1.390(5)	C(81)-C(86)	1.392(5)
C(82)-C(83)	1.384(5)	C(83)-C(84)	1.375(6)
C(84)-C(85)	1.382(6)	C(85)-C(86)	1.388(5)
C(87)-C(92)	1.387(5)	C(87)-C(88)	1.393(5)
C(88)-C(89)	1.386(5)	C(89)-C(90)	1.372(5)
C(90)-C(91)	1.375(5)	C(91)-C(92)	1.385(5)
H(1)-Ru(1)-C(1)	83.9	H(1)-Ru(1)-F(1)	92.4
C(1)-Ru(1)-F(1)	174.71(12)	H(1)-Ru(1)-P(3)	85.6
C(1)-Ru(1)-P(3)	93.95(11)	F(1)-Ru(1)-P(3)	81.98(6)
H(1)-Ru(1)-P(1)	82.6	C(1)-Ru(1)-P(1)	86.35(11)
F(1)-Ru(1)-P(1)	96.94(6)	P(3)-Ru(1)-P(1)	168.09(3)
H(1)-Ru(1)-P(2)	173.2	C(1)-Ru(1)-P(2)	102.79(11)
F(1)-Ru(1)-P(2)	80.85(6)	P(3)-Ru(1)-P(2)	92.64(3)
P(1)-Ru(1)-P(2)	98.92(3)	H(2)-Ru(2)-C(47)	88.3
H(2)-Ru(2)-F(2)	86.4	C(47)-Ru(2)-F(2)	173.39(12)
H(2)-Ru(2)-P(5)	84.4	C(47)-Ru(2)-P(5)	93.05(11)
F(2)-Ru(2)-P(5)	82.48(6)	H(2)-Ru(2)-P(4)	86.9
C(47)-Ru(2)-P(4)	85.23(11)	F(2)-Ru(2)-P(4)	98.44(6)

P(5)-Ru(2)-P(4)	171.20(3)	H(2)-Ru(2)-P(6)	167.3
C(47)-Ru(2)-P(6)	103.89(11)	F(2)-Ru(2)-P(6)	81.18(6)
P(5)-Ru(2)-P(6)	91.40(3)	P(4)-Ru(2)-P(6)	97.39(3)
C(14)-P(1)-C(8)	103.98(16)	C(14)-P(1)-C(2)	102.00(16)
C(8)-P(1)-C(2)	98.15(16)	C(14)-P(1)-Ru(1)	117.31(12)
C(8)-P(1)-Ru(1)	119.29(12)	C(2)-P(1)-Ru(1)	113.17(12)
C(23)-P(2)-C(29)	104.12(16)	C(23)-P(2)-C(20)	101.45(17)
C(29)-P(2)-C(20)	98.35(16)	C(23)-P(2)-Ru(1)	122.50(12)
C(29)-P(2)-Ru(1)	117.26(12)	C(20)-P(2)-Ru(1)	109.47(12)
C(35)-P(3)-C(22)	105.72(17)	C(35)-P(3)-C(41)	102.29(16)
C(22)-P(3)-C(41)	99.00(16)	C(35)-P(3)-Ru(1)	117.18(12)
C(22)-P(3)-Ru(1)	114.79(12)	C(41)-P(3)-Ru(1)	115.57(11)
C(60)-P(4)-C(48)	106.55(16)	C(60)-P(4)-C(54)	101.63(15)
C(48)-P(4)-C(54)	98.89(15)	C(60)-P(4)-Ru(2)	115.40(11)
C(48)-P(4)-Ru(2)	118.99(11)	C(54)-P(4)-Ru(2)	112.86(11)
C(75)-P(5)-C(69)	102.24(16)	C(75)-P(5)-C(66)	106.72(17)
C(69)-P(5)-C(66)	97.10(16)	C(75)-P(5)-Ru(2)	113.82(12)
C(69)-P(5)-Ru(2)	118.62(12)	C(66)-P(5)-Ru(2)	116.15(12)
C(81)-P(6)-C(87)	105.18(16)	C(81)-P(6)-C(68)	98.01(15)
C(87)-P(6)-C(68)	100.42(16)	C(81)-P(6)-Ru(2)	117.41(11)
C(87)-P(6)-Ru(2)	122.40(11)	C(68)-P(6)-Ru(2)	109.43(12)
O(1)-C(1)-Ru(1)	177.2(3)	C(3)-C(2)-C(7)	118.3(3)
C(3)-C(2)-P(1)	123.6(3)	C(7)-C(2)-P(1)	117.8(3)
C(2)-C(3)-C(4)	120.4(4)	C(5)-C(4)-C(3)	120.2(4)
C(6)-C(5)-C(4)	119.6(4)	C(7)-C(6)-C(5)	120.2(4)
C(6)-C(7)-C(2)	121.4(4)	C(13)-C(8)-C(9)	119.4(3)
C(13)-C(8)-P(1)	120.7(3)	C(9)-C(8)-P(1)	120.0(3)
C(10)-C(9)-C(8)	120.3(3)	C(11)-C(10)-C(9)	120.1(4)
C(10)-C(11)-C(12)	119.8(4)	C(11)-C(12)-C(13)	120.6(4)
C(8)-C(13)-C(12)	119.8(4)	C(15)-C(14)-C(19)	118.5(3)
C(15)-C(14)-P(1)	124.0(3)	C(19)-C(14)-P(1)	117.4(3)
C(14)-C(15)-C(16)	120.7(4)	C(17)-C(16)-C(15)	119.9(4)
C(18)-C(17)-C(16)	120.4(3)	C(17)-C(18)-C(19)	120.0(4)
C(18)-C(19)-C(14)	120.5(3)	C(21)-C(20)-P(2)	114.2(3)
C(20)-C(21)-C(22)	113.4(3)	C(21)-C(22)-P(3)	118.3(2)
C(24)-C(23)-C(28)	118.0(3)	C(24)-C(23)-P(2)	121.5(3)
C(28)-C(23)-P(2)	120.5(3)	C(25)-C(24)-C(23)	121.1(4)
C(26)-C(25)-C(24)	120.2(4)	C(25)-C(26)-C(27)	119.8(4)
C(26)-C(27)-C(28)	120.1(4)	C(27)-C(28)-C(23)	120.7(4)
C(30)-C(29)-C(34)	118.3(3)	C(30)-C(29)-P(2)	124.6(3)
C(34)-C(29)-P(2)	117.0(3)	C(31)-C(30)-C(29)	121.5(4)
C(32)-C(31)-C(30)	119.5(4)	C(31)-C(32)-C(33)	120.1(4)
C(34)-C(33)-C(32)	120.2(4)	C(33)-C(34)-C(29)	120.3(4)
C(36)-C(35)-C(40)	119.0(4)	C(36)-C(35)-P(3)	118.4(3)
C(40)-C(35)-P(3)	122.6(3)	C(35)-C(36)-C(37)	120.5(4)
C(38)-C(37)-C(36)	120.3(5)	C(37)-C(38)-C(39)	119.9(4)
C(38)-C(39)-C(40)	120.6(4)	C(39)-C(40)-C(35)	119.5(4)
C(42)-C(41)-C(46)	118.4(3)	C(42)-C(41)-P(3)	122.3(3)
C(46)-C(41)-P(3)	119.2(3)	C(43)-C(42)-C(41)	120.8(3)
C(44)-C(43)-C(42)	120.1(4)	C(43)-C(44)-C(45)	119.9(3)
C(44)-C(45)-C(46)	120.3(3)	C(45)-C(46)-C(41)	120.5(3)
O(2)-C(47)-Ru(2)	176.6(3)	C(53)-C(48)-C(49)	117.9(3)
C(53)-C(48)-P(4)	118.3(3)	C(49)-C(48)-P(4)	123.4(3)
C(50)-C(49)-C(48)	121.0(4)	C(51)-C(50)-C(49)	120.3(4)
C(50)-C(51)-C(52)	119.6(4)	C(51)-C(52)-C(53)	120.6(4)

C(52)-C(53)-C(48)	120.5(4)	C(59)-C(54)-C(55)	118.0(3)
C(59)-C(54)-P(4)	118.4(3)	C(55)-C(54)-P(4)	123.5(3)
C(54)-C(55)-C(56)	120.4(4)	C(57)-C(56)-C(55)	120.6(4)
C(56)-C(57)-C(58)	119.9(3)	C(57)-C(58)-C(59)	119.6(4)
C(54)-C(59)-C(58)	121.5(3)	C(61)-C(60)-C(65)	117.7(3)
C(61)-C(60)-P(4)	124.6(3)	C(65)-C(60)-P(4)	117.7(3)
C(62)-C(61)-C(60)	120.8(4)	C(63)-C(62)-C(61)	120.6(4)
C(64)-C(63)-C(62)	119.7(4)	C(63)-C(64)-C(65)	119.7(4)
C(64)-C(65)-C(60)	121.4(3)	C(67)-C(66)-P(5)	119.8(2)
C(68)-C(67)-C(66)	113.8(3)	C(67)-C(68)-P(6)	114.6(2)
C(70)-C(69)-C(74)	118.6(4)	C(70)-C(69)-P(5)	119.9(3)
C(74)-C(69)-P(5)	121.0(3)	C(69)-C(70)-C(71)	120.5(4)
C(72)-C(71)-C(70)	120.0(4)	C(71)-C(72)-C(73)	120.2(4)
C(72)-C(73)-C(74)	120.0(4)	C(73)-C(74)-C(69)	120.8(4)
C(80)-C(75)-C(76)	118.2(3)	C(80)-C(75)-P(5)	123.8(3)
C(76)-C(75)-P(5)	117.9(3)	C(77)-C(76)-C(75)	120.9(4)
C(78)-C(77)-C(76)	119.9(4)	C(79)-C(78)-C(77)	119.8(4)
C(78)-C(79)-C(80)	120.8(4)	C(75)-C(80)-C(79)	120.3(4)
C(82)-C(81)-C(86)	118.3(3)	C(82)-C(81)-P(6)	116.9(3)
C(86)-C(81)-P(6)	124.8(3)	C(83)-C(82)-C(81)	120.9(4)
C(84)-C(83)-C(82)	120.4(4)	C(83)-C(84)-C(85)	119.5(4)
C(84)-C(85)-C(86)	120.4(4)	C(85)-C(86)-C(81)	120.5(4)
C(92)-C(87)-C(88)	117.8(3)	C(92)-C(87)-P(6)	121.6(3)
C(88)-C(87)-P(6)	120.4(3)	C(89)-C(88)-C(87)	120.7(3)
C(90)-C(89)-C(88)	120.6(4)	C(89)-C(90)-C(91)	119.5(4)
C(90)-C(91)-C(92)	120.3(4)	C(91)-C(92)-C(87)	121.1(3)

Table 88. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(dppp)(PPh_3)(CO)HF **(62)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	22(1)	21(1)	26(1)	2(1)	1(1)	0(1)
Ru(2)	22(1)	21(1)	25(1)	2(1)	-1(1)	2(1)
P(1)	24(1)	22(1)	28(1)	1(1)	1(1)	2(1)
P(2)	23(1)	23(1)	31(1)	3(1)	2(1)	-1(1)
P(3)	24(1)	26(1)	26(1)	1(1)	-1(1)	2(1)
P(4)	25(1)	21(1)	26(1)	1(1)	0(1)	2(1)
P(5)	26(1)	25(1)	26(1)	1(1)	0(1)	1(1)
P(6)	23(1)	21(1)	27(1)	2(1)	0(1)	2(1)
F(1)	29(1)	24(1)	31(1)	6(1)	0(1)	0(1)
F(2)	30(1)	23(1)	34(1)	3(1)	2(1)	2(1)
O(1)	43(2)	28(1)	41(2)	11(1)	4(1)	-1(1)
O(2)	48(2)	29(2)	39(2)	10(1)	-5(1)	5(1)
C(1)	24(2)	28(2)	28(2)	-1(2)	2(1)	0(2)
C(2)	28(2)	25(2)	30(2)	4(2)	-2(2)	-3(2)
C(3)	30(2)	28(2)	40(2)	3(2)	1(2)	0(2)
C(4)	50(3)	23(2)	48(2)	0(2)	-7(2)	-3(2)
C(5)	33(2)	41(2)	48(2)	7(2)	-3(2)	-11(2)
C(6)	28(2)	41(2)	48(2)	-2(2)	1(2)	-6(2)
C(7)	28(2)	31(2)	41(2)	-3(2)	2(2)	-3(2)
C(8)	24(2)	32(2)	28(2)	3(2)	1(2)	2(2)
C(9)	38(2)	29(2)	34(2)	-3(2)	2(2)	3(2)
C(10)	35(2)	42(2)	29(2)	-4(2)	-1(2)	-1(2)

C(11)	33(2)	50(3)	34(2)	6(2)	-2(2)	5(2)
C(12)	48(3)	32(2)	43(2)	6(2)	-9(2)	6(2)
C(13)	35(2)	28(2)	39(2)	1(2)	-6(2)	3(2)
C(14)	22(2)	24(2)	37(2)	0(2)	1(2)	-1(1)
C(15)	34(2)	32(2)	38(2)	7(2)	8(2)	5(2)
C(16)	40(2)	48(3)	44(2)	3(2)	17(2)	9(2)
C(17)	36(2)	36(2)	55(3)	2(2)	15(2)	10(2)
C(18)	27(2)	23(2)	53(2)	6(2)	2(2)	2(2)
C(19)	28(2)	27(2)	36(2)	2(2)	1(2)	1(2)
C(20)	27(2)	25(2)	40(2)	3(2)	4(2)	-2(2)
C(21)	30(2)	28(2)	42(2)	0(2)	-3(2)	-6(2)
C(22)	31(2)	27(2)	36(2)	-4(2)	-1(2)	1(2)
C(23)	23(2)	29(2)	31(2)	2(2)	3(2)	2(2)
C(24)	27(2)	34(2)	47(2)	9(2)	-1(2)	-4(2)
C(25)	23(2)	48(3)	57(3)	12(2)	-5(2)	-4(2)
C(26)	34(2)	41(2)	49(2)	8(2)	-9(2)	5(2)
C(27)	41(3)	40(2)	50(3)	15(2)	-5(2)	-4(2)
C(28)	29(2)	36(2)	43(2)	9(2)	-3(2)	-6(2)
C(29)	28(2)	26(2)	33(2)	1(2)	5(2)	-6(2)
C(30)	35(2)	29(2)	40(2)	-3(2)	6(2)	0(2)
C(31)	42(3)	38(2)	46(2)	-6(2)	15(2)	0(2)
C(32)	57(3)	46(3)	35(2)	-5(2)	18(2)	-12(2)
C(33)	61(3)	40(2)	39(2)	9(2)	3(2)	-3(2)
C(34)	35(2)	35(2)	36(2)	4(2)	2(2)	2(2)
C(35)	31(2)	32(2)	29(2)	-2(2)	-3(2)	12(2)
C(36)	45(2)	36(2)	33(2)	4(2)	0(2)	6(2)
C(37)	73(3)	41(2)	32(2)	6(2)	8(2)	17(2)
C(38)	73(3)	56(3)	32(2)	9(2)	4(2)	36(3)
C(39)	48(3)	72(3)	32(2)	-5(2)	-8(2)	28(3)
C(40)	39(2)	53(3)	32(2)	-2(2)	-1(2)	13(2)
C(41)	24(2)	22(2)	32(2)	0(1)	2(2)	-1(1)
C(42)	35(2)	42(2)	29(2)	-1(2)	-3(2)	8(2)
C(43)	38(2)	44(2)	34(2)	-5(2)	4(2)	7(2)
C(44)	26(2)	31(2)	45(2)	-2(2)	0(2)	4(2)
C(45)	27(2)	32(2)	38(2)	5(2)	-5(2)	4(2)
C(46)	34(2)	31(2)	30(2)	2(2)	2(2)	1(2)
C(47)	29(2)	29(2)	25(2)	-2(2)	-3(2)	4(2)
C(48)	23(2)	24(2)	31(2)	4(2)	-2(1)	1(1)
C(49)	39(2)	32(2)	34(2)	0(2)	4(2)	-1(2)
C(50)	36(2)	46(2)	29(2)	1(2)	3(2)	3(2)
C(51)	39(2)	40(2)	34(2)	12(2)	5(2)	6(2)
C(52)	55(3)	31(2)	43(2)	8(2)	11(2)	-1(2)
C(53)	46(2)	31(2)	33(2)	2(2)	6(2)	-2(2)
C(54)	28(2)	24(2)	28(2)	3(2)	4(2)	2(2)
C(55)	30(2)	27(2)	42(2)	-1(2)	0(2)	2(2)
C(56)	41(2)	24(2)	44(2)	-2(2)	-1(2)	6(2)
C(57)	36(2)	33(2)	34(2)	4(2)	5(2)	10(2)
C(58)	25(2)	37(2)	46(2)	1(2)	-2(2)	4(2)
C(59)	28(2)	24(2)	43(2)	-4(2)	1(2)	2(2)
C(60)	25(2)	25(2)	27(2)	0(1)	2(1)	4(1)
C(61)	34(2)	44(2)	33(2)	10(2)	-1(2)	-7(2)
C(62)	40(3)	66(3)	31(2)	11(2)	-11(2)	-13(2)
C(63)	32(2)	40(2)	43(2)	-4(2)	-3(2)	-9(2)
C(64)	28(2)	31(2)	41(2)	7(2)	3(2)	-2(2)
C(65)	30(2)	31(2)	28(2)	4(2)	-3(2)	0(2)

C(66)	35(2)	24(2)	34(2)	-4(2)	-2(2)	5(2)
C(67)	28(2)	30(2)	37(2)	-2(2)	4(2)	7(2)
C(68)	26(2)	22(2)	35(2)	3(2)	2(2)	4(1)
C(69)	30(2)	27(2)	33(2)	2(2)	-5(2)	-1(2)
C(70)	31(2)	33(2)	44(2)	1(2)	-1(2)	-3(2)
C(71)	32(2)	38(2)	59(3)	4(2)	3(2)	-3(2)
C(72)	32(2)	41(2)	63(3)	7(2)	-15(2)	-4(2)
C(73)	60(3)	53(3)	42(3)	0(2)	-21(2)	-14(2)
C(74)	47(3)	51(3)	32(2)	5(2)	-7(2)	-12(2)
C(75)	36(2)	31(2)	25(2)	-1(2)	-2(2)	-6(2)
C(76)	43(2)	40(2)	30(2)	4(2)	0(2)	5(2)
C(77)	62(3)	41(2)	34(2)	11(2)	-6(2)	2(2)
C(78)	72(3)	48(3)	30(2)	10(2)	-5(2)	-19(2)
C(79)	53(3)	57(3)	36(2)	3(2)	7(2)	-10(2)
C(80)	36(2)	44(2)	33(2)	1(2)	2(2)	-3(2)
C(81)	25(2)	27(2)	28(2)	1(2)	-3(1)	5(2)
C(82)	40(2)	35(2)	36(2)	6(2)	-1(2)	-4(2)
C(83)	62(3)	46(3)	34(2)	11(2)	-5(2)	0(2)
C(84)	58(3)	48(3)	34(2)	4(2)	-14(2)	6(2)
C(85)	45(3)	48(3)	45(3)	-9(2)	-18(2)	2(2)
C(86)	35(2)	36(2)	36(2)	2(2)	-1(2)	0(2)
C(87)	24(2)	29(2)	27(2)	3(2)	1(1)	-1(2)
C(88)	35(2)	32(2)	41(2)	6(2)	8(2)	11(2)
C(89)	47(3)	29(2)	50(2)	13(2)	16(2)	7(2)
C(90)	38(2)	32(2)	41(2)	5(2)	11(2)	-4(2)
C(91)	27(2)	46(2)	44(2)	6(2)	6(2)	1(2)
C(92)	30(2)	41(2)	43(2)	12(2)	1(2)	2(2)

Table 89. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(dppp)(PPh_3)(CO)HF **(62)**

Atom	x	y	z	
H(3)	1806	1450	3438	39
H(4)	3499	2398	3411	49
H(5)	5533	2008	3065	49
H(6)	5832	687	2702	47
H(7)	4156	-249	2720	40
H(9)	2875	372	4264	41
H(10)	3896	-130	5078	43
H(11)	4168	-1503	5100	47
H(12)	3330	-2377	4328	49
H(13)	2229	-1886	3523	42
H(15)	400	-41	4314	41
H(16)	-1330	747	4651	52
H(17)	-2518	1502	4017	50
H(18)	-2030	1453	3041	41
H(19)	-306	671	2697	36
H(20A)	-942	-2823	2442	37
H(20B)	-2429	-2607	2276	37
H(21A)	-1643	-2344	1313	40
H(21B)	-1801	-3259	1443	40
H(22A)	184	-3178	1031	38
H(22B)	519	-3266	1704	38
H(24)	-3922	-1689	2124	43

H(25)	-5521	-1090	1562	51
H(26)	-4988	14	1075	50
H(27)	-2849	533	1158	52
H(28)	-1235	-67	1716	43
H(30)	-3286	-646	3058	42
H(31)	-4032	-694	3991	51
H(32)	-2888	-1423	4656	56
H(33)	-1007	-2117	4383	56
H(34)	-279	-2086	3447	43
H(36)	2569	-834	888	45
H(37)	2272	-246	13	58
H(38)	491	-617	-624	64
H(39)	-973	-1604	-403	62
H(40)	-678	-2226	464	50
H(42)	2774	-2619	463	43
H(43)	4728	-3315	350	46
H(44)	5929	-3690	1164	41
H(45)	5177	-3371	2093	39
H(46)	3263	-2639	2214	38
H(49)	-3130	-4831	4579	42
H(50)	-4046	-5457	5329	44
H(51)	-4779	-6780	5174	44
H(52)	-4508	-7498	4276	51
H(53)	-3479	-6906	3537	44
H(55)	-2727	-3585	3658	40
H(56)	-4388	-2640	3600	44
H(57)	-6476	-3023	3231	41
H(58)	-6924	-4360	2898	43
H(59)	-5269	-5304	2948	39
H(61)	-871	-5102	4433	44
H(62)	1003	-4332	4706	55
H(63)	1864	-3485	4069	47
H(64)	910	-3463	3131	39
H(65)	-929	-4260	2846	36
H(66A)	-1849	-8177	1683	38
H(66B)	-1541	-7952	1047	38
H(67A)	433	-8148	1534	38
H(67B)	359	-7216	1442	38
H(68A)	1161	-7564	2409	33
H(68B)	-330	-7790	2516	33
H(70)	-4770	-7449	2153	43
H(71)	-6615	-8284	1898	52
H(72)	-7083	-8743	930	55
H(73)	-5695	-8410	213	63
H(74)	-3850	-7597	462	52
H(76)	-4073	-5703	1028	45
H(77)	-3807	-4858	293	55
H(78)	-1917	-4925	-236	60
H(79)	-346	-5872	-60	59
H(80)	-608	-6741	664	45
H(82)	-785	-7129	3548	44
H(83)	84	-7260	4485	56
H(84)	2056	-6621	4813	57
H(85)	3147	-5830	4200	57
H(86)	2260	-5671	3266	43

H(88)	-65	-5038	1868	43
H(89)	1443	-4440	1309	49
H(90)	3569	-4914	1256	44
H(91)	4197	-5990	1772	47
H(92)	2697	-6599	2327	45
H(1)	2665	-1102	2280	26(9)
H(2)	-3851	-6162	2411	71(14)

Table 90. Crystal data and structure refinement for $[Ru(dppp)_2(CO)H/F][SiF_5]$ **(63/64)**.

Compound	$[Ru(dppp)_2(CO)H/F][SiF_5]$ **(63/64)**
Empirical formula	C67 H64.70 F5.30 O P4 Ru Si
Formula weight	1239.63
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/n
Unit cell dimensions	a = 12.9230(1)Å α = 90°
	b = 17.5000(1)Å β = 92.343(1)°
	c = 26.1850(2)Å γ = 90°
Volume	5916.85(7) $Å^3$
Z	4
Density (calculated)	1.392 Mg/m^3
Absorption coefficient	0.453 mm^{-1}
F(000)	2562
Crystal size	0.50 x 0.40 x 0.35 mm
Theta range for data collection	3.58 to 30.03°
Index ranges	-18<=h<=18; -24<=k<=24; -36<=l<=36
Reflections collected	110956
Independent reflections	17278 [R(int) = 0.0726]
Reflections observed (>2σ)	12060
Data Completeness	0.998
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.92 and 0.83
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17278 / 2 / 716
Goodness-of-fit on F^2	1.023
Final R indices [I>2σ(I)]	R^1 = 0.0451 wR_2 = 0.1061
R indices (all data)	R^1 = 0.0808 wR_2 = 0.1224
Largest diff. peak and hole	0.810 and -0.980 $eÅ^{-3}$

Table 91. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Ru(dppp)_2(CO)H/F][SiF_5]$ **(63/64)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	9120(1)	2815(1)	3669(1)	20(1)
P(1)	7916(1)	3831(1)	3759(1)	23(1)
P(2)	10427(1)	3729(1)	3909(1)	24(1)
P(3)	10284(1)	1764(1)	3543(1)	23(1)
P(4)	7786(1)	1863(1)	3697(1)	22(1)
Si(1)	4328(1)	2767(1)	1102(1)	78(1)
F(1)	9201(5)	2657(4)	4432(3)	57(2)
F(2)	3115(3)	2567(4)	1118(2)	223(3)

F(3)	5455(3)	3040(4)	1172(2)	209(3)
F(4)	4479(5)	1946(2)	1268(2)	214(3)
F(5)	4207(2)	2920(2)	522(1)	110(1)
F(6)	4004(6)	3381(3)	1493(2)	248(3)
O(3)	9140(2)	3147(1)	2527(1)	38(1)
C(1)	9117(2)	3012(1)	2958(1)	26(1)
C(2)	8504(2)	4758(1)	3606(1)	28(1)
C(3)	9188(2)	5076(1)	4052(1)	32(1)
C(4)	9925(2)	4495(1)	4316(1)	29(1)
C(5)	6788(2)	3824(1)	3313(1)	28(1)
C(6)	5806(2)	3632(2)	3474(1)	37(1)
C(7)	4967(2)	3616(2)	3122(1)	49(1)
C(8)	5092(3)	3767(2)	2618(1)	52(1)
C(9)	6066(3)	3958(2)	2451(1)	45(1)
C(10)	6905(2)	3999(1)	2797(1)	34(1)
C(11)	7367(2)	4065(1)	4371(1)	29(1)
C(12)	7701(2)	3710(2)	4823(1)	33(1)
C(13)	7359(3)	3970(2)	5289(1)	47(1)
C(14)	6690(3)	4583(2)	5304(1)	54(1)
C(15)	6343(2)	4940(2)	4856(1)	46(1)
C(16)	6682(2)	4686(2)	4390(1)	36(1)
C(17)	11106(2)	4265(1)	3424(1)	28(1)
C(18)	11428(2)	5019(2)	3516(1)	34(1)
C(19)	11960(2)	5417(2)	3150(1)	42(1)
C(20)	12207(2)	5068(2)	2697(1)	44(1)
C(21)	11914(2)	4317(2)	2607(1)	40(1)
C(22)	11358(2)	3926(2)	2966(1)	33(1)
C(23)	11496(2)	3409(1)	4338(1)	33(1)
C(24)	11278(3)	3162(2)	4825(1)	47(1)
C(25)	12092(3)	2977(2)	5174(1)	62(1)
C(26)	13102(3)	3032(2)	5028(2)	69(1)
C(27)	13316(3)	3276(2)	4548(2)	63(1)
C(28)	12523(2)	3467(2)	4202(1)	43(1)
C(29)	9606(2)	1031(1)	3147(1)	28(1)
C(30)	8888(2)	515(1)	3443(1)	34(1)
C(31)	8308(2)	917(1)	3866(1)	28(1)
C(32)	11411(2)	1928(1)	3156(1)	26(1)
C(33)	12412(2)	1961(2)	3381(1)	34(1)
C(34)	13252(2)	2087(2)	3079(1)	43(1)
C(35)	13115(2)	2203(2)	2558(1)	42(1)
C(36)	12130(2)	2175(2)	2334(1)	36(1)
C(37)	11279(2)	2027(1)	2629(1)	30(1)
C(38)	10821(2)	1181(1)	4072(1)	28(1)
C(39)	10631(2)	1346(2)	4575(1)	36(1)
C(40)	10976(3)	856(2)	4965(1)	49(1)
C(41)	11511(3)	196(2)	4846(1)	52(1)
C(42)	11704(2)	25(2)	4344(1)	47(1)
C(43)	11367(2)	518(2)	3956(1)	37(1)
C(44)	6878(2)	1928(1)	4215(1)	27(1)
C(45)	7278(2)	1875(2)	4719(1)	34(1)
C(46)	6618(3)	1832(2)	5124(1)	44(1)
C(47)	5561(3)	1832(2)	5030(1)	51(1)
C(48)	5155(2)	1885(2)	4536(1)	48(1)
C(49)	5809(2)	1939(2)	4129(1)	35(1)
C(50)	6946(2)	1627(1)	3136(1)	26(1)

C(51)	6343(2)	966(2)	3128(1)	35(1)
C(52)	5704(2)	789(2)	2706(1)	39(1)
C(53)	5654(2)	1270(2)	2285(1)	34(1)
C(54)	6244(2)	1922(2)	2286(1)	32(1)
C(55)	6894(2)	2099(1)	2709(1)	27(1)
C(56)	9482(3)	690(2)	1796(1)	44(1)
C(57)	10330(3)	870(2)	1521(1)	53(1)
C(58)	10365(3)	1555(2)	1262(1)	66(1)
C(59)	9543(4)	2054(2)	1281(1)	69(1)
C(60)	8697(3)	1864(2)	1552(1)	57(1)
C(61)	8666(2)	1186(2)	1810(1)	45(1)
C(62)	9871(3)	4134(2)	1515(1)	58(1)
C(63)	10494(3)	4600(2)	1240(1)	61(1)
C(64)	10137(4)	4925(2)	795(2)	71(1)
C(65)	9153(4)	4781(2)	612(1)	76(1)
C(66)	8510(3)	4299(2)	882(2)	69(1)
C(67)	8878(3)	3979(2)	1344(1)	59(1)

Table 92. Bond lengths [Å] and angles [°] for $[Ru(dppp)_2(CO)H/F][SiF_5]$ **(63/64)**.

Ru(1)-C(1)	1.895(2)	Ru(1)-F(1)	2.015(7)
Ru(1)-P(1)	2.3793(6)	Ru(1)-P(2)	2.3911(6)
Ru(1)-P(4)	2.4014(6)	Ru(1)-P(3)	2.4076(6)
P(1)-C(11)	1.825(2)	P(1)-C(5)	1.829(2)
P(1)-C(2)	1.843(2)	P(2)-C(17)	1.832(3)
P(2)-C(23)	1.832(3)	P(2)-C(4)	1.846(2)
P(3)-C(32)	1.831(2)	P(3)-C(38)	1.833(2)
P(3)-C(29)	1.848(2)	P(4)-C(44)	1.833(2)
P(4)-C(31)	1.834(2)	P(4)-C(50)	1.839(2)
Si(1)-F(4)	1.512(4)	Si(1)-F(3)	1.537(4)
Si(1)-F(5)	1.542(2)	Si(1)-F(6)	1.553(5)
Si(1)-F(2)	1.608(4)	O(3)-C(1)	1.154(3)
C(2)-C(3)	1.539(3)	C(3)-C(4)	1.538(4)
C(5)-C(6)	1.395(4)	C(5)-C(10)	1.401(4)
C(6)-C(7)	1.394(4)	C(7)-C(8)	1.364(5)
C(8)-C(9)	1.389(5)	C(9)-C(10)	1.385(4)
C(11)-C(12)	1.391(4)	C(11)-C(16)	1.403(4)
C(12)-C(13)	1.391(4)	C(13)-C(14)	1.379(5)
C(14)-C(15)	1.386(5)	C(15)-C(16)	1.388(4)
C(17)-C(22)	1.390(4)	C(17)-C(18)	1.401(3)
C(18)-C(19)	1.388(4)	C(19)-C(20)	1.384(4)
C(20)-C(21)	1.384(4)	C(21)-C(22)	1.387(4)
C(23)-C(24)	1.386(4)	C(23)-C(28)	1.391(4)
C(24)-C(25)	1.403(4)	C(25)-C(26)	1.379(6)
C(26)-C(27)	1.365(6)	C(27)-C(28)	1.380(4)
C(29)-C(30)	1.527(4)	C(30)-C(31)	1.535(3)
C(32)-C(37)	1.396(3)	C(32)-C(33)	1.399(3)
C(33)-C(34)	1.387(4)	C(34)-C(35)	1.382(4)
C(35)-C(36)	1.382(4)	C(36)-C(37)	1.394(4)
C(38)-C(39)	1.380(4)	C(38)-C(43)	1.397(4)
C(39)-C(40)	1.394(4)	C(40)-C(41)	1.388(5)
C(41)-C(42)	1.381(5)	C(42)-C(43)	1.390(4)
C(44)-C(49)	1.391(4)	C(44)-C(45)	1.400(4)
C(45)-C(46)	1.389(4)	C(46)-C(47)	1.378(5)
C(47)-C(48)	1.379(5)	C(48)-C(49)	1.392(4)

C(50)-C(55)	1.390(3)	C(50)-C(51)	1.394(3)
C(51)-C(52)	1.389(4)	C(52)-C(53)	1.385(4)
C(53)-C(54)	1.373(4)	C(54)-C(55)	1.396(3)
C(56)-C(61)	1.367(4)	C(56)-C(57)	1.373(5)
C(57)-C(58)	1.378(5)	C(58)-C(59)	1.378(6)
C(59)-C(60)	1.368(5)	C(60)-C(61)	1.366(5)
C(62)-C(67)	1.370(5)	C(62)-C(63)	1.371(5)
C(63)-C(64)	1.361(5)	C(64)-C(65)	1.363(6)
C(65)-C(66)	1.396(6)	C(66)-C(67)	1.397(5)
C(1)-Ru(1)-F(1)	176.2(2)	C(1)-Ru(1)-P(1)	89.24(7)
F(1)-Ru(1)-P(1)	90.75(19)	C(1)-Ru(1)-P(2)	96.32(7)
F(1)-Ru(1)-P(2)	79.86(19)	P(1)-Ru(1)-P(2)	86.14(2)
C(1)-Ru(1)-P(4)	100.57(7)	F(1)-Ru(1)-P(4)	83.26(19)
P(1)-Ru(1)-P(4)	92.43(2)	P(2)-Ru(1)-P(4)	163.03(2)
C(1)-Ru(1)-P(3)	88.83(7)	F(1)-Ru(1)-P(3)	91.33(19)
P(1)-Ru(1)-P(3)	177.11(2)	P(2)-Ru(1)-P(3)	96.21(2)
P(4)-Ru(1)-P(3)	85.81(2)	C(11)-P(1)-C(5)	103.47(12)
C(11)-P(1)-C(2)	99.86(11)	C(5)-P(1)-C(2)	101.10(11)
C(11)-P(1)-Ru(1)	122.23(9)	C(5)-P(1)-Ru(1)	116.07(8)
C(2)-P(1)-Ru(1)	111.04(8)	C(17)-P(2)-C(23)	102.15(12)
C(17)-P(2)-C(4)	102.57(12)	C(23)-P(2)-C(4)	98.20(12)
C(17)-P(2)-Ru(1)	120.91(8)	C(23)-P(2)-Ru(1)	117.65(9)
C(4)-P(2)-Ru(1)	112.06(8)	C(32)-P(3)-C(38)	102.69(11)
C(32)-P(3)-C(29)	99.67(11)	C(38)-P(3)-C(29)	101.16(12)
C(32)-P(3)-Ru(1)	118.15(8)	C(38)-P(3)-Ru(1)	122.79(8)
C(29)-P(3)-Ru(1)	108.83(8)	C(44)-P(4)-C(31)	96.78(11)
C(44)-P(4)-C(50)	103.39(11)	C(31)-P(4)-C(50)	100.94(11)
C(44)-P(4)-Ru(1)	117.46(8)	C(31)-P(4)-Ru(1)	112.10(8)
C(50)-P(4)-Ru(1)	122.16(8)	F(4)-Si(1)-F(3)	98.7(3)
F(4)-Si(1)-F(5)	117.0(2)	F(3)-Si(1)-F(5)	96.95(19)
F(4)-Si(1)-F(6)	120.2(3)	F(3)-Si(1)-F(6)	89.1(3)
F(5)-Si(1)-F(6)	120.7(3)	F(4)-Si(1)-F(2)	84.3(3)
F(3)-Si(1)-F(2)	169.9(3)	F(5)-Si(1)-F(2)	90.24(18)
F(6)-Si(1)-F(2)	81.0(3)	O(3)-C(1)-Ru(1)	177.9(2)
C(3)-C(2)-P(1)	112.51(17)	C(4)-C(3)-C(2)	115.3(2)
C(3)-C(4)-P(2)	116.56(17)	C(6)-C(5)-C(10)	118.7(2)
C(6)-C(5)-P(1)	121.4(2)	C(10)-C(5)-P(1)	120.0(2)
C(7)-C(6)-C(5)	119.9(3)	C(8)-C(7)-C(6)	121.1(3)
C(7)-C(8)-C(9)	119.7(3)	C(10)-C(9)-C(8)	120.2(3)
C(9)-C(10)-C(5)	120.4(3)	C(12)-C(11)-C(16)	119.3(2)
C(12)-C(11)-P(1)	122.0(2)	C(16)-C(11)-P(1)	118.3(2)
C(13)-C(12)-C(11)	120.2(3)	C(14)-C(13)-C(12)	120.0(3)
C(13)-C(14)-C(15)	120.6(3)	C(14)-C(15)-C(16)	119.8(3)
C(15)-C(16)-C(11)	120.1(3)	C(22)-C(17)-C(18)	118.2(2)
C(22)-C(17)-P(2)	121.01(19)	C(18)-C(17)-P(2)	120.7(2)
C(19)-C(18)-C(17)	120.4(3)	C(20)-C(19)-C(18)	120.5(3)
C(21)-C(20)-C(19)	119.6(3)	C(20)-C(21)-C(22)	120.0(3)
C(21)-C(22)-C(17)	121.3(3)	C(24)-C(23)-C(28)	119.3(3)
C(24)-C(23)-P(2)	118.8(2)	C(28)-C(23)-P(2)	121.6(2)
C(23)-C(24)-C(25)	119.7(3)	C(26)-C(25)-C(24)	119.7(4)
C(27)-C(26)-C(25)	120.5(3)	C(26)-C(27)-C(28)	120.4(4)
C(27)-C(28)-C(23)	120.3(3)	C(30)-C(29)-P(3)	114.16(17)
C(29)-C(30)-C(31)	114.9(2)	C(30)-C(31)-P(4)	115.13(17)
C(37)-C(32)-C(33)	119.0(2)	C(37)-C(32)-P(3)	119.92(19)

C(33)-C(32)-P(3)	121.10(19)	C(34)-C(33)-C(32)	119.9(3)
C(35)-C(34)-C(33)	120.9(3)	C(36)-C(35)-C(34)	119.6(3)
C(35)-C(36)-C(37)	120.3(3)	C(36)-C(37)-C(32)	120.3(2)
C(39)-C(38)-C(43)	119.5(2)	C(39)-C(38)-P(3)	121.8(2)
C(43)-C(38)-P(3)	118.46(19)	C(38)-C(39)-C(40)	120.5(3)
C(41)-C(40)-C(39)	119.6(3)	C(42)-C(41)-C(40)	120.4(3)
C(41)-C(42)-C(43)	119.8(3)	C(42)-C(43)-C(38)	120.2(3)
C(49)-C(44)-C(45)	118.7(2)	C(49)-C(44)-P(4)	122.8(2)
C(45)-C(44)-P(4)	118.12(19)	C(46)-C(45)-C(44)	120.6(3)
C(47)-C(46)-C(45)	119.9(3)	C(46)-C(47)-C(48)	120.3(3)
C(47)-C(48)-C(49)	120.2(3)	C(44)-C(49)-C(48)	120.3(3)
C(55)-C(50)-C(51)	118.3(2)	C(55)-C(50)-P(4)	121.14(18)
C(51)-C(50)-P(4)	120.54(19)	C(52)-C(51)-C(50)	120.7(2)
C(53)-C(52)-C(51)	120.3(2)	C(54)-C(53)-C(52)	119.7(2)
C(53)-C(54)-C(55)	120.2(2)	C(50)-C(55)-C(54)	120.8(2)
C(61)-C(56)-C(57)	120.1(3)	C(56)-C(57)-C(58)	120.0(3)
C(57)-C(58)-C(59)	119.5(3)	C(60)-C(59)-C(58)	119.8(3)
C(61)-C(60)-C(59)	120.5(3)	C(60)-C(61)-C(56)	120.0(3)
C(67)-C(62)-C(63)	120.5(4)	C(64)-C(63)-C(62)	120.9(4)
C(63)-C(64)-C(65)	120.1(4)	C(64)-C(65)-C(66)	120.0(4)
C(65)-C(66)-C(67)	119.5(4)	C(62)-C(67)-C(66)	119.0(4)

Table 93. Anisotropic displacement parameters ($Å^2$ x 10^3) for $[Ru(dppp)_2(CO)H/F][SiF_5]$ **(63/64)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}$ U11 + ... + 2 h k a* b* U

Ru(1)	21(1)	19(1)	20(1)	1(1)	1(1)	0(1)
P(1)	24(1)	21(1)	24(1)	2(1)	2(1)	1(1)
P(2)	24(1)	22(1)	26(1)	-1(1)	-2(1)	-1(1)
P(3)	23(1)	23(1)	22(1)	0(1)	1(1)	2(1)
P(4)	23(1)	21(1)	21(1)	1(1)	1(1)	-3(1)
Si(1)	99(1)	90(1)	42(1)	17(1)	-18(1)	-16(1)
F(2)	117(3)	452(9)	101(3)	38(4)	21(2)	-2(4)
F(3)	128(3)	381(7)	114(3)	92(4)	-58(3)	-98(4)
F(4)	362(7)	103(3)	170(4)	73(3)	-98(4)	14(4)
F(5)	85(2)	201(3)	43(1)	39(2)	-17(1)	-31(2)
F(6)	403(10)	215(6)	129(4)	-58(4)	26(5)	-42(6)
O(3)	38(1)	49(1)	27(1)	5(1)	2(1)	0(1)
C(1)	22(1)	23(1)	31(1)	0(1)	0(1)	0(1)
C(2)	29(1)	21(1)	35(1)	2(1)	4(1)	1(1)
C(3)	32(1)	23(1)	40(1)	-4(1)	4(1)	-3(1)
C(4)	33(1)	25(1)	29(1)	-5(1)	0(1)	-3(1)
C(5)	30(1)	20(1)	34(1)	1(1)	-5(1)	3(1)
C(6)	32(1)	28(1)	51(2)	5(1)	-3(1)	-1(1)
C(7)	32(2)	33(2)	80(2)	4(2)	-13(2)	-5(1)
C(8)	50(2)	31(2)	72(2)	5(2)	-32(2)	-2(1)
C(9)	67(2)	25(1)	40(2)	7(1)	-22(1)	3(1)
C(10)	43(2)	24(1)	36(1)	3(1)	-6(1)	2(1)
C(11)	29(1)	26(1)	32(1)	-2(1)	6(1)	-3(1)
C(12)	42(2)	29(1)	29(1)	-1(1)	8(1)	-3(1)
C(13)	67(2)	43(2)	32(2)	1(1)	15(1)	-4(2)
C(14)	72(2)	47(2)	45(2)	-11(2)	28(2)	-2(2)
C(15)	46(2)	40(2)	54(2)	-9(1)	21(1)	6(1)
C(16)	34(1)	33(1)	41(2)	-2(1)	9(1)	3(1)

C(17)	23(1)	26(1)	34(1)	1(1)	-1(1)	-3(1)
C(18)	26(1)	29(1)	47(2)	-1(1)	2(1)	-3(1)
C(19)	35(2)	27(1)	63(2)	8(1)	5(1)	-8(1)
C(20)	36(2)	43(2)	54(2)	17(1)	6(1)	-10(1)
C(21)	37(2)	46(2)	38(2)	3(1)	7(1)	-2(1)
C(22)	31(1)	32(1)	37(1)	1(1)	2(1)	-3(1)
C(23)	37(1)	23(1)	40(1)	-5(1)	-12(1)	1(1)
C(24)	54(2)	45(2)	40(2)	1(1)	-15(1)	1(2)
C(25)	84(3)	52(2)	49(2)	0(2)	-29(2)	11(2)
C(26)	61(2)	51(2)	91(3)	-5(2)	-45(2)	14(2)
C(27)	42(2)	44(2)	100(3)	1(2)	-29(2)	6(2)
C(28)	36(2)	29(1)	63(2)	-2(1)	-12(1)	6(1)
C(29)	30(1)	26(1)	28(1)	-6(1)	2(1)	1(1)
C(30)	34(1)	23(1)	45(2)	-3(1)	2(1)	0(1)
C(31)	29(1)	23(1)	31(1)	5(1)	2(1)	-2(1)
C(32)	25(1)	22(1)	30(1)	-3(1)	4(1)	0(1)
C(33)	30(1)	31(1)	41(2)	-1(1)	-2(1)	-2(1)
C(34)	26(1)	43(2)	61(2)	-1(1)	2(1)	-4(1)
C(35)	36(2)	35(2)	57(2)	-5(1)	20(1)	-4(1)
C(36)	45(2)	31(1)	35(1)	-4(1)	15(1)	1(1)
C(37)	32(1)	29(1)	29(1)	-2(1)	5(1)	1(1)
C(38)	28(1)	28(1)	29(1)	6(1)	-1(1)	2(1)
C(39)	35(1)	41(2)	30(1)	4(1)	-4(1)	4(1)
C(40)	52(2)	63(2)	31(2)	12(1)	-4(1)	3(2)
C(41)	50(2)	55(2)	51(2)	26(2)	-6(2)	9(2)
C(42)	48(2)	38(2)	55(2)	14(1)	-3(2)	12(1)
C(43)	40(2)	32(1)	39(2)	6(1)	2(1)	7(1)
C(44)	30(1)	22(1)	30(1)	-1(1)	7(1)	-2(1)
C(45)	42(2)	31(1)	29(1)	3(1)	7(1)	-4(1)
C(46)	70(2)	34(2)	30(1)	-1(1)	18(1)	-7(1)
C(47)	63(2)	37(2)	57(2)	-8(2)	36(2)	-6(2)
C(48)	38(2)	40(2)	67(2)	-10(2)	23(2)	-3(1)
C(49)	31(1)	29(1)	45(2)	-4(1)	8(1)	-2(1)
C(50)	24(1)	27(1)	25(1)	-1(1)	-2(1)	-1(1)
C(51)	40(2)	32(1)	33(1)	4(1)	-3(1)	-11(1)
C(52)	40(2)	36(2)	41(2)	-5(1)	-5(1)	-15(1)
C(53)	30(1)	38(2)	33(1)	-9(1)	-5(1)	-1(1)
C(54)	33(1)	37(1)	27(1)	0(1)	-4(1)	3(1)
C(55)	26(1)	27(1)	28(1)	-1(1)	0(1)	0(1)
C(56)	57(2)	34(2)	41(2)	-8(1)	-6(1)	-6(1)
C(57)	45(2)	58(2)	56(2)	-22(2)	-5(2)	2(2)
C(58)	79(3)	66(3)	54(2)	-21(2)	33(2)	-23(2)
C(59)	135(4)	35(2)	40(2)	0(1)	24(2)	4(2)
C(60)	76(2)	52(2)	43(2)	-8(2)	2(2)	24(2)
C(61)	46(2)	45(2)	45(2)	-17(1)	5(1)	-11(1)
C(62)	81(3)	48(2)	46(2)	8(2)	2(2)	7(2)
C(63)	79(3)	52(2)	52(2)	-1(2)	15(2)	3(2)
C(64)	110(4)	55(2)	52(2)	11(2)	34(2)	28(2)
C(65)	124(4)	66(3)	39(2)	3(2)	13(2)	55(3)
C(66)	85(3)	53(2)	67(2)	-21(2)	-10(2)	32(2)
C(67)	81(3)	34(2)	61(2)	3(2)	2(2)	10(2)

Table 94. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Ru(dppp)_2(CO)H/F][SiF_5]$ **(63/64)**.

Atom	x	y	z	U(eq)
H(2A)	8930	4698	3303	34
H(2B)	7948	5130	3519	34
H(3A)	9606	5502	3922	38
H(3B)	8731	5289	4311	38
H(4A)	9558	4253	4598	35
H(4B)	10522	4777	4470	35
H(6)	5709	3513	3823	45
H(7)	4296	3498	3236	58
H(8)	4517	3742	2381	62
H(9)	6157	4060	2100	54
H(10)	7564	4148	2683	41
H(12)	8164	3290	4814	40
H(13)	7586	3725	5598	56
H(14)	6464	4761	5623	65
H(15)	5875	5357	4869	55
H(16)	6451	4932	4083	43
H(18)	11281	5260	3830	41
H(19)	12156	5933	3212	50
H(20)	12576	5341	2449	53
H(21)	12093	4071	2300	48
H(22)	11144	3415	2897	40
H(24)	10580	3118	4922	56
H(25)	11948	2815	5510	75
H(26)	13653	2900	5262	83
H(27)	14015	3314	4452	75
H(28)	12679	3638	3870	52
H(29A)	9194	1290	2871	34
H(29B)	10129	709	2984	34
H(30A)	9304	94	3598	40
H(30B)	8373	286	3198	40
H(31A)	8786	972	4170	33
H(31B)	7729	585	3965	33
H(33)	12515	1897	3740	41
H(34)	13931	2094	3232	52
H(35)	13695	2302	2357	50
H(36)	12032	2258	1976	44
H(37)	10606	1992	2470	36
H(39)	10262	1796	4655	43
H(40)	10845	972	5311	59
H(41)	11747	-140	5111	62
H(42)	12067	-430	4264	56
H(43)	11507	405	3611	44
H(45)	8006	1870	4785	40
H(46)	6895	1802	5465	53
H(47)	5110	1796	5307	62
H(48)	4425	1884	4474	57
H(49)	5525	1984	3790	42
H(51)	6369	634	3416	42
H(52)	5299	335	2705	47
H(53)	5214	1149	1997	41

H(54)	6211	2253	1999	39
H(55)	7305	2549	2705	32
H(56)	9462	220	1977	53
H(57)	10893	523	1509	64
H(58)	10952	1682	1072	79
H(59)	9563	2529	1106	83
H(60)	8128	2206	1562	68
H(61)	8077	1058	1998	54
H(62)	10131	3917	1827	70
H(63)	11184	4696	1361	73
H(64)	10573	5254	611	86
H(65)	8906	5008	301	91
H(66)	7828	4191	754	83
H(67)	8446	3658	1535	71

Table 95. Crystal data and structure refinement for Ru(IMes)(dppp)(CO)HF **(68)**.

Compound	Ru(IMes)(dppp)(CO)HF **(68)**
Empirical formula	C56 H59 F N2 O P2 Ru
Formula weight	958.06
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.7800(1)Å α = 96.084(1)^{o}
	b = 12.1130(2)Å β = 97.792(1)^{o}
	c = 17.1580(2)Å γ = 97.116(1)^{o}
Volume	2388.16(5) Å^3
Z	2
Density (calculated)	1.332 Mg/m^3
Absorption coefficient	0.441 mm^{-1}
F(000)	1000
Crystal size	0.35 x 0.22 x 0.15 mm
Theta range for data collection	3.53 to 27.48 ^{o}.
Index ranges	-15<=h<=15; -15<=k<=15; -22<=l<=22
Reflections collected	42981
Independent reflections	10884 [R(int) = 0.0278]
Reflections observed (>2σ)	9977
Data Completeness	0.994
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.92 and 0.90
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10884 / 1 / 577
Goodness-of-fit on F^2	1.072
Final R indices [I>2σ(I)]	R1 = 0.0279 wR2 = 0.0679
R indices (all data)	R1 = 0.0320 wR2 = 0.0709
Largest diff. peak and hole	0.691 and -0.649 eÅ^{-3}

Table 96. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ru(IMes)(dppp)(CO)HF **(68)**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	4856(1)	2843(1)	7881(1)	16(1)
P(1)	6867(1)	2947(1)	8080(1)	18(1)
P(2)	4668(1)	1639(1)	6631(1)	18(1)
F(1)	4951(1)	1282(1)	8361(1)	24(1)
O(1)	5080(1)	5028(1)	7225(1)	29(1)
N(1)	2743(1)	2439(1)	8779(1)	20(1)
N(2)	2116(1)	3004(1)	7679(1)	21(1)
C(1)	4945(1)	4170(1)	7474(1)	21(1)
C(2)	3115(1)	2756(1)	8099(1)	19(1)
C(3)	1570(1)	2494(2)	8772(1)	26(1)
C(4)	1178(1)	2846(2)	8087(1)	28(1)
C(5)	3423(1)	2278(1)	9519(1)	20(1)
C(6)	3809(1)	3232(1)	10072(1)	22(1)
C(7)	4376(1)	3075(2)	10813(1)	25(1)
C(8)	4531(2)	2013(2)	11009(1)	27(1)
C(9)	4098(2)	1089(2)	10453(1)	28(1)
C(10)	3526(2)	1198(1)	9701(1)	25(1)
C(11)	3574(2)	4379(1)	9890(1)	26(1)
C(12)	5128(2)	1864(2)	11823(1)	35(1)
C(13)	3013(2)	172(2)	9136(1)	33(1)
C(14)	2005(1)	3530(2)	6962(1)	22(1)
C(15)	1429(1)	2912(2)	6256(1)	28(1)
C(16)	1322(2)	3476(2)	5582(1)	38(1)
C(17)	1738(2)	4599(2)	5607(1)	39(1)
C(18)	2229(2)	5198(2)	6332(1)	35(1)
C(19)	2346(1)	4686(2)	7024(1)	27(1)
C(20)	880(2)	1718(2)	6225(1)	37(1)
C(21)	1636(2)	5183(3)	4868(1)	60(1)
C(22)	2736(2)	5378(2)	7816(1)	34(1)
C(23)	7553(1)	3045(1)	9118(1)	21(1)
C(24)	8733(2)	3438(2)	9340(1)	29(1)
C(25)	9260(2)	3459(2)	10117(1)	35(1)
C(26)	8617(2)	3088(2)	10677(1)	33(1)
C(27)	7451(2)	2707(2)	10466(1)	30(1)
C(28)	6914(2)	2677(1)	9689(1)	24(1)
C(29)	7755(1)	4119(1)	7769(1)	23(1)
C(30)	8560(1)	4000(2)	7249(1)	30(1)
C(31)	9286(2)	4931(2)	7107(1)	41(1)
C(32)	9205(2)	5980(2)	7468(1)	48(1)
C(33)	8404(2)	6114(2)	7980(1)	44(1)
C(34)	7681(2)	5191(2)	8125(1)	31(1)
C(35)	7451(1)	1704(1)	7691(1)	23(1)
C(36)	7034(1)	1281(1)	6813(1)	24(1)
C(37)	5781(1)	696(1)	6654(1)	22(1)
C(38)	4786(1)	2271(1)	5719(1)	21(1)
C(39)	4226(1)	3203(1)	5593(1)	24(1)
C(40)	4281(2)	3702(2)	4903(1)	29(1)
C(41)	4908(2)	3296(2)	4335(1)	31(1)
C(42)	5465(2)	2372(2)	4453(1)	32(1)

C(43)	5399(2)	1860(2)	5135(1)	27(1)
C(44)	3432(1)	521(1)	6325(1)	23(1)
C(45)	3091(2)	-105(2)	6913(1)	30(1)
C(46)	2248(2)	-1040(2)	6718(1)	39(1)
C(47)	1732(2)	-1350(2)	5939(1)	42(1)
C(48)	2045(2)	-722(2)	5357(1)	38(1)
C(49)	2894(2)	210(2)	5544(1)	30(1)
C(50)	9322(2)	-114(2)	8901(2)	62(1)
C(51)	8895(2)	-589(2)	8045(1)	40(1)
C(52)	7794(2)	-1179(2)	7830(1)	39(1)
C(53)	7388(2)	-1634(2)	7053(1)	43(1)
C(54)	8074(2)	-1495(2)	6474(1)	46(1)
C(55)	9165(2)	-887(2)	6676(2)	52(1)
C(56)	9574(2)	-442(2)	7457(2)	51(1)

Table 97. Bond lengths [Å] and angles [°] for Ru(IMes)(dppp)(CO)HF **(68)**.

Ru(1)-C(1)	1.8162(17)	C(18)-C(19)	1.394(2)
Ru(1)-C(2)	2.1270(15)	C(19)-C(22)	1.501(3)
Ru(1)-F(1)	2.1501(10)	C(23)-C(28)	1.390(2)
Ru(1)-P(1)	2.3323(4)	C(23)-C(24)	1.399(2)
Ru(1)-P(2)	2.4287(4)	C(24)-C(25)	1.389(2)
P(1)-C(29)	1.8279(17)	C(25)-C(26)	1.381(3)
P(1)-C(35)	1.8314(16)	C(26)-C(27)	1.380(3)
P(1)-C(23)	1.8396(16)	C(27)-C(28)	1.391(2)
P(2)-C(38)	1.8295(16)	C(29)-C(34)	1.393(3)
P(2)-C(44)	1.8387(17)	C(29)-C(30)	1.396(2)
P(2)-C(37)	1.8413(16)	C(30)-C(31)	1.393(3)
O(1)-C(1)	1.166(2)	C(31)-C(32)	1.374(3)
N(1)-C(2)	1.376(2)	C(32)-C(33)	1.387(3)
N(1)-C(3)	1.390(2)	C(33)-C(34)	1.385(3)
N(1)-C(5)	1.4504(19)	C(35)-C(36)	1.532(2)
N(2)-C(2)	1.3776(19)	C(36)-C(37)	1.531(2)
N(2)-C(4)	1.391(2)	C(38)-C(39)	1.397(2)
N(2)-C(14)	1.442(2)	C(38)-C(43)	1.397(2)
C(3)-C(4)	1.335(2)	C(39)-C(40)	1.391(2)
C(5)-C(10)	1.392(2)	C(40)-C(41)	1.386(3)
C(5)-C(6)	1.401(2)	C(41)-C(42)	1.385(3)
C(6)-C(7)	1.396(2)	C(42)-C(43)	1.388(2)
C(6)-C(11)	1.507(2)	C(44)-C(49)	1.393(2)
C(7)-C(8)	1.392(3)	C(44)-C(45)	1.397(2)
C(8)-C(9)	1.387(3)	C(45)-C(46)	1.390(3)
C(8)-C(12)	1.515(2)	C(46)-C(47)	1.384(3)
C(9)-C(10)	1.399(2)	C(47)-C(48)	1.380(3)
C(10)-C(13)	1.501(2)	C(48)-C(49)	1.391(3)
C(14)-C(15)	1.396(2)	C(50)-C(51)	1.513(3)
C(14)-C(19)	1.397(3)	C(51)-C(56)	1.383(3)
C(15)-C(16)	1.403(3)	C(51)-C(52)	1.383(3)
C(15)-C(20)	1.501(3)	C(52)-C(53)	1.385(3)
C(16)-C(17)	1.382(3)	C(53)-C(54)	1.373(3)
C(17)-C(18)	1.385(3)	C(54)-C(55)	1.380(3)
C(17)-C(21)	1.514(3)	C(55)-C(56)	1.387(4)
C(1)-Ru(1)-C(2)	97.54(6)	C(16)-C(15)-C(20)	121.14(17)
C(1)-Ru(1)-F(1)	173.76(5)	C(17)-C(16)-C(15)	122.40(18)

C(2)-Ru(1)-F(1)	88.63(5)	C(16)-C(17)-C(18)	118.49(17)
C(1)-Ru(1)-P(1)	91.22(5)	C(16)-C(17)-C(21)	121.4(2)
C(2)-Ru(1)-P(1)	161.64(4)	C(18)-C(17)-C(21)	120.1(2)
F(1)-Ru(1)-P(1)	82.59(3)	C(17)-C(18)-C(19)	121.67(19)
C(1)-Ru(1)-P(2)	97.09(5)	C(18)-C(19)-C(14)	118.03(17)
C(2)-Ru(1)-P(2)	102.49(4)	C(18)-C(19)-C(22)	120.52(18)
F(1)-Ru(1)-P(2)	82.43(3)	C(14)-C(19)-C(22)	121.27(16)
P(1)-Ru(1)-P(2)	92.340(14)	C(28)-C(23)-C(24)	119.02(15)
C(29)-P(1)-C(35)	104.30(8)	C(28)-C(23)-P(1)	120.16(12)
C(29)-P(1)-C(23)	99.41(7)	C(24)-C(23)-P(1)	120.75(12)
C(35)-P(1)-C(23)	98.06(7)	C(25)-C(24)-C(23)	120.61(16)
C(29)-P(1)-Ru(1)	119.84(5)	C(26)-C(25)-C(24)	119.84(17)
C(35)-P(1)-Ru(1)	116.26(6)	C(27)-C(26)-C(25)	119.95(16)
C(23)-P(1)-Ru(1)	115.57(5)	C(26)-C(27)-C(28)	120.74(17)
C(38)-P(2)-C(44)	102.64(7)	C(23)-C(28)-C(27)	119.84(16)
C(38)-P(2)-C(37)	103.25(7)	C(34)-C(29)-C(30)	118.46(17)
C(44)-P(2)-C(37)	95.52(7)	C(34)-C(29)-P(1)	117.12(13)
C(38)-P(2)-Ru(1)	119.37(5)	C(30)-C(29)-P(1)	124.22(14)
C(44)-P(2)-Ru(1)	120.99(5)	C(31)-C(30)-C(29)	120.43(19)
C(37)-P(2)-Ru(1)	111.30(5)	C(32)-C(31)-C(30)	120.2(2)
C(2)-N(1)-C(3)	111.79(13)	C(31)-C(32)-C(33)	120.05(19)
C(2)-N(1)-C(5)	129.06(13)	C(34)-C(33)-C(32)	120.0(2)
C(3)-N(1)-C(5)	118.00(13)	C(33)-C(34)-C(29)	120.86(19)
C(2)-N(2)-C(4)	111.98(13)	C(36)-C(35)-P(1)	115.51(11)
C(2)-N(2)-C(14)	127.52(13)	C(37)-C(36)-C(35)	112.97(14)
C(4)-N(2)-C(14)	119.86(13)	C(36)-C(37)-P(2)	115.28(11)
O(1)-C(1)-Ru(1)	175.60(14)	C(39)-C(38)-C(43)	118.26(15)
N(1)-C(2)-N(2)	102.35(13)	C(39)-C(38)-P(2)	118.56(12)
N(1)-C(2)-Ru(1)	124.24(11)	C(43)-C(38)-P(2)	123.18(13)
N(2)-C(2)-Ru(1)	133.37(11)	C(40)-C(39)-C(38)	120.51(16)
C(4)-C(3)-N(1)	107.16(15)	C(41)-C(40)-C(39)	120.56(16)
C(3)-C(4)-N(2)	106.71(14)	C(42)-C(41)-C(40)	119.40(16)
C(10)-C(5)-C(6)	122.33(15)	C(41)-C(42)-C(43)	120.28(17)
C(10)-C(5)-N(1)	119.98(14)	C(42)-C(43)-C(38)	120.97(16)
C(6)-C(5)-N(1)	117.01(14)	C(49)-C(44)-C(45)	118.96(16)
C(7)-C(6)-C(5)	117.62(15)	C(49)-C(44)-P(2)	124.23(14)
C(7)-C(6)-C(11)	121.00(15)	C(45)-C(44)-P(2)	116.59(13)
C(5)-C(6)-C(11)	121.32(14)	C(46)-C(45)-C(44)	120.42(18)
C(8)-C(7)-C(6)	121.72(16)	C(47)-C(46)-C(45)	120.1(2)
C(9)-C(8)-C(7)	118.70(15)	C(48)-C(47)-C(46)	119.90(18)
C(9)-C(8)-C(12)	120.55(17)	C(47)-C(48)-C(49)	120.49(18)
C(7)-C(8)-C(12)	120.72(17)	C(48)-C(49)-C(44)	120.14(18)
C(8)-C(9)-C(10)	121.89(16)	C(56)-C(51)-C(52)	118.1(2)
C(5)-C(10)-C(9)	117.62(16)	C(56)-C(51)-C(50)	121.8(2)
C(5)-C(10)-C(13)	122.36(15)	C(52)-C(51)-C(50)	120.1(2)
C(9)-C(10)-C(13)	119.98(16)	C(51)-C(52)-C(53)	121.2(2)
C(15)-C(14)-C(19)	121.92(16)	C(54)-C(53)-C(52)	120.2(2)
C(15)-C(14)-N(2)	119.57(16)	C(53)-C(54)-C(55)	119.2(2)
C(19)-C(14)-N(2)	117.96(15)	C(54)-C(55)-C(56)	120.4(2)
C(14)-C(15)-C(16)	117.00(18)	C(51)-C(56)-C(55)	120.8(2)
C(14)-C(15)-C(20)	121.75(16)		

Table 98. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(IMes)(dppp)(CO)HF **(68)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	15(1)	18(1)	15(1)	0(1)	1(1)	4(1)
P(1)	16(1)	21(1)	17(1)	1(1)	2(1)	5(1)
P(2)	19(1)	20(1)	16(1)	-1(1)	1(1)	5(1)
F(1)	21(1)	30(1)	19(1)	-5(1)	5(1)	-5(1)
O(1)	31(1)	24(1)	32(1)	9(1)	1(1)	5(1)
N(1)	18(1)	24(1)	18(1)	2(1)	3(1)	3(1)
N(2)	15(1)	28(1)	19(1)	2(1)	1(1)	5(1)
C(1)	17(1)	27(1)	18(1)	-2(1)	1(1)	6(1)
C(2)	18(1)	17(1)	20(1)	-1(1)	2(1)	3(1)
C(3)	18(1)	36(1)	26(1)	4(1)	5(1)	2(1)
C(4)	15(1)	41(1)	28(1)	5(1)	4(1)	4(1)
C(5)	19(1)	26(1)	17(1)	4(1)	4(1)	6(1)
C(6)	20(1)	26(1)	20(1)	1(1)	5(1)	5(1)
C(7)	23(1)	32(1)	19(1)	1(1)	4(1)	5(1)
C(8)	22(1)	40(1)	21(1)	8(1)	6(1)	7(1)
C(9)	29(1)	30(1)	29(1)	11(1)	8(1)	9(1)
C(10)	25(1)	26(1)	24(1)	4(1)	7(1)	4(1)
C(11)	30(1)	25(1)	24(1)	0(1)	2(1)	7(1)
C(12)	32(1)	52(1)	24(1)	13(1)	4(1)	8(1)
C(13)	41(1)	23(1)	33(1)	2(1)	5(1)	3(1)
C(14)	15(1)	34(1)	19(1)	4(1)	1(1)	9(1)
C(15)	18(1)	41(1)	24(1)	-2(1)	0(1)	11(1)
C(16)	25(1)	68(1)	20(1)	1(1)	-2(1)	17(1)
C(17)	27(1)	63(1)	33(1)	20(1)	7(1)	20(1)
C(18)	26(1)	43(1)	41(1)	18(1)	8(1)	14(1)
C(19)	18(1)	35(1)	29(1)	6(1)	4(1)	9(1)
C(20)	25(1)	42(1)	39(1)	-10(1)	-4(1)	7(1)
C(21)	51(1)	102(2)	41(1)	39(1)	8(1)	32(1)
C(22)	33(1)	30(1)	38(1)	-2(1)	5(1)	7(1)
C(23)	21(1)	22(1)	18(1)	0(1)	0(1)	7(1)
C(24)	21(1)	42(1)	24(1)	5(1)	2(1)	5(1)
C(25)	23(1)	48(1)	29(1)	1(1)	-6(1)	2(1)
C(26)	35(1)	43(1)	20(1)	2(1)	-4(1)	10(1)
C(27)	34(1)	35(1)	21(1)	6(1)	4(1)	6(1)
C(28)	23(1)	27(1)	23(1)	4(1)	2(1)	5(1)
C(29)	17(1)	28(1)	22(1)	6(1)	-2(1)	3(1)
C(30)	20(1)	45(1)	24(1)	10(1)	0(1)	3(1)
C(31)	22(1)	69(2)	31(1)	22(1)	-2(1)	-6(1)
C(32)	36(1)	54(1)	48(1)	29(1)	-12(1)	-16(1)
C(33)	44(1)	30(1)	52(1)	13(1)	-10(1)	-2(1)
C(34)	28(1)	28(1)	37(1)	6(1)	-1(1)	4(1)
C(35)	21(1)	25(1)	24(1)	1(1)	1(1)	10(1)
C(36)	22(1)	28(1)	22(1)	-2(1)	3(1)	10(1)
C(37)	25(1)	21(1)	22(1)	-1(1)	2(1)	7(1)
C(38)	22(1)	23(1)	18(1)	-1(1)	1(1)	2(1)
C(39)	24(1)	26(1)	22(1)	0(1)	2(1)	5(1)
C(40)	30(1)	27(1)	28(1)	6(1)	1(1)	6(1)
C(41)	35(1)	35(1)	23(1)	7(1)	4(1)	0(1)

C(42)	34(1)	40(1)	23(1)	3(1)	10(1)	7(1)
C(43)	29(1)	30(1)	23(1)	0(1)	5(1)	9(1)
C(44)	19(1)	23(1)	26(1)	-3(1)	2(1)	6(1)
C(45)	25(1)	31(1)	33(1)	3(1)	4(1)	4(1)
C(46)	29(1)	34(1)	53(1)	6(1)	10(1)	1(1)
C(47)	23(1)	35(1)	62(1)	-13(1)	5(1)	-3(1)
C(48)	23(1)	47(1)	38(1)	-19(1)	-1(1)	4(1)
C(49)	25(1)	36(1)	26(1)	-6(1)	1(1)	7(1)
C(50)	52(2)	65(2)	61(2)	6(1)	-10(1)	-1(1)
C(51)	31(1)	35(1)	55(1)	10(1)	3(1)	8(1)
C(52)	34(1)	37(1)	48(1)	11(1)	8(1)	5(1)
C(53)	37(1)	39(1)	52(1)	8(1)	2(1)	3(1)
C(54)	52(1)	40(1)	48(1)	6(1)	8(1)	19(1)
C(55)	46(1)	57(1)	65(2)	16(1)	26(1)	20(1)
C(56)	28(1)	53(1)	73(2)	12(1)	11(1)	5(1)

Table 99. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Ru(IMes)(dppp)(CO)HF **(68)**.

Atom	x	y	z	U(eq)
H(3)	1130	2314	9177	32
H(4)	407	2965	7913	34
H(7)	4662	3711	11193	30
H(9)	4194	361	10585	33
H(11A)	3930	4939	10339	39
H(11B)	2737	4393	9799	39
H(11C)	3901	4552	9414	39
H(12A)	5965	1924	11822	53
H(12B)	4841	1123	11957	53
H(12C)	4964	2446	12217	53
H(13A)	2437	371	8726	49
H(13B)	2640	-391	9425	49
H(13C)	3626	-136	8886	49
H(16)	950	3071	5090	45
H(18)	2492	5976	6359	42
H(20A)	1389	1319	6559	55
H(20B)	759	1353	5677	55
H(20C)	134	1704	6419	55
H(21A)	1598	4631	4400	90
H(21B)	2313	5753	4898	90
H(21C)	933	5541	4827	90
H(22A)	2095	5348	8126	51
H(22B)	2980	6157	7739	51
H(22C)	3387	5080	8100	51
H(24)	9177	3693	8955	35
H(25)	10061	3729	10262	42
H(26)	8977	3095	11208	39
H(27)	7009	2462	10855	36
H(28)	6112	2405	9548	29
H(30)	8611	3278	6990	36
H(31)	9840	4840	6760	49
H(32)	9697	6614	7366	57
H(33)	8350	6839	8232	52
H(34)	7128	5289	8472	38

H(35A)	8306	1876	7771	28
H(35B)	7247	1090	8006	28
H(36A)	7099	1924	6502	29
H(36B)	7544	751	6627	29
H(37A)	5668	202	7069	27
H(37B)	5661	213	6139	27
H(39)	3804	3497	5982	29
H(40)	3884	4327	4820	34
H(41)	4956	3648	3869	37
H(42)	5895	2088	4065	38
H(43)	5775	1220	5205	32
H(45)	3438	109	7449	36
H(46)	2026	-1466	7120	46
H(47)	1163	-1995	5804	51
H(48)	1677	-927	4824	46
H(49)	3106	636	5139	36
H(50A)	10169	-39	9001	93
H(50B)	8998	-619	9250	93
H(50C)	9076	624	9006	93
H(52)	7307	-1274	8223	46
H(53)	6633	-2044	6919	52
H(54)	7800	-1812	5942	55
H(55)	9640	-774	6278	63
H(56)	10329	-31	7588	61
H(1)	5027	3551	8696	28(5)

Table 100. Crystal data and structure refinement for $[Ru(dppp)_2(CO)_2(\mu\text{-}F)_3][SiF_5]$ **(71)**

Compound	$[Ru(dppp)_2(CO)_2(\mu\text{-}F)_3][SiF_5]$ **(71)**
Empirical formula	C58.50 H56 Cl5 F8 O2 P4 Ru2 Si
Formula weight	1474.39
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 12.9680(2)Å α = 101.777(1)°
	b = 14.3480(2)Å β = 99.119(1)°
	c = 18.4620(2)Å γ = 105.422(1)°
Volume	3158.27(7) $Å^3$
Z	2
Density (calculated)	1.550 Mg/m^3
Absorption coefficient	0.874 mm^{-1}
F(000)	1484
Crystal size	0.35 x 0.25 x 0.20 mm
Theta range for data collection	3.54 to 27.48°
Index ranges	-16<=h<=16; -18<=k<=18; -23<=l<=23
Reflections collected	58179
Independent reflections	14416 [R(int) = 0.0407]
Reflections observed (>2σ)	11606
Data Completeness	0.995
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.88 and 0.83
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14416 / 0 / 739
Goodness-of-fit on F^2	1.048
Final R indices [I>2σ(I)]	R1 = 0.0533 wR2 = 0.1467
R indices (all data)	R1 = 0.0691 wR2 = 0.1561
Largest diff. peak and hole	2.080 and -1.119 $eÅ^{-3}$

Table 101. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $[Ru(dppp)_2(CO)_2(\mu\text{-}F)_3][SiF_5]$ **(71)**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	11089(1)	5068(1)	3602(1)	27(1)
Ru(2)	9090(1)	3383(1)	2666(1)	26(1)
Cl(2)	6776(4)	8250(3)	2383(3)	151(2)
Cl(3)	5497(4)	1342(3)	4013(3)	153(2)
Cl(5)	5426(1)	6908(1)	-340(1)	84(1)
Cl(6)	7536(2)	8218(2)	580(1)	98(1)
P(1)	11987(1)	6443(1)	3244(1)	33(1)
P(2)	12681(1)	4901(1)	4194(1)	31(1)
P(3)	8145(1)	3239(1)	1470(1)	29(1)
P(4)	8898(1)	1727(1)	2389(1)	32(1)
Si(1)	5884(1)	77(1)	-1442(1)	51(1)
F(1)	9496(2)	4959(2)	3029(1)	34(1)
F(2)	10729(2)	3985(2)	2557(1)	28(1)
F(3)	10134(2)	3720(2)	3750(1)	43(1)
F(4)	6793(5)	320(5)	-700(3)	134(2)
F(38)	5593(6)	-1044(4)	-1459(4)	152(3)

F(52)	5254(4)	774(4)	-1077(3)	109(2)
F(71)	4939(4)	-390(7)	-2202(3)	162(3)
F(91)	6723(4)	578(4)	-1866(3)	108(2)
O(2)	7001(3)	2863(3)	3173(2)	46(1)
O(90)	11145(3)	6530(3)	5014(2)	49(1)
C(1)	11136(4)	5953(3)	4472(2)	37(1)
C(2)	7798(3)	3054(3)	2957(2)	34(1)
C(3)	13174(4)	7299(3)	3975(3)	44(1)
C(4)	14042(4)	6827(3)	4232(3)	44(1)
C(5)	13717(4)	6090(3)	4716(2)	41(1)
C(6)	6973(3)	2102(3)	1073(2)	36(1)
C(7)	7235(4)	1109(3)	1056(3)	41(1)
C(8)	7541(4)	920(3)	1837(3)	41(1)
C(9)	12569(3)	6245(3)	2409(2)	35(1)
C(10)	12835(4)	5383(3)	2175(2)	39(1)
C(11)	13400(4)	5276(4)	1596(3)	49(1)
C(12)	13672(4)	6048(4)	1241(3)	48(1)
C(13)	13372(4)	6900(4)	1451(3)	52(1)
C(14)	12830(4)	7004(4)	2041(3)	46(1)
C(15)	11114(4)	7211(3)	3041(3)	41(1)
C(16)	10145(4)	6773(4)	2495(3)	51(1)
C(17)	9432(5)	7299(4)	2337(4)	59(1)
C(18)	9669(7)	8283(6)	2735(4)	79(2)
C(19)	10650(10)	8742(6)	3271(5)	107(3)
C(20)	11370(7)	8201(4)	3426(4)	78(2)
C(21)	13377(3)	4229(3)	3599(2)	34(1)
C(22)	12758(4)	3337(3)	3071(2)	39(1)
C(23)	13273(4)	2771(4)	2637(3)	50(1)
C(24)	14404(4)	3104(4)	2726(3)	54(1)
C(25)	15024(4)	3983(4)	3243(3)	50(1)
C(26)	14518(3)	4552(4)	3678(2)	39(1)
C(27)	12511(3)	4205(3)	4921(2)	35(1)
C(28)	11886(4)	4415(4)	5443(3)	50(1)
C(29)	11782(5)	3913(5)	6007(3)	59(1)
C(30)	12288(4)	3190(4)	6050(3)	51(1)
C(31)	12917(4)	2980(4)	5543(3)	48(1)
C(32)	13023(4)	3481(3)	4977(3)	41(1)
C(34)	7520(3)	4234(3)	1407(2)	32(1)
C(35)	7459(4)	4611(3)	772(2)	39(1)
C(36)	6944(4)	5336(4)	715(3)	43(1)
C(37)	6474(4)	5682(3)	1292(3)	42(1)
C(38)	6520(4)	5314(4)	1926(3)	52(1)
C(39)	7053(4)	4598(4)	1986(3)	46(1)
C(40)	8964(3)	3304(3)	758(2)	32(1)
C(41)	8633(4)	2639(4)	38(2)	42(1)
C(42)	9288(5)	2757(4)	-489(3)	51(1)
C(43)	10253(5)	3508(5)	-306(3)	55(1)
C(44)	10592(4)	4184(4)	408(3)	48(1)
C(45)	9954(3)	4076(3)	937(2)	38(1)
C(46)	9815(4)	1292(3)	1849(3)	41(1)
C(47)	9849(6)	320(4)	1766(4)	75(2)
C(48)	10453(7)	-48(5)	1291(5)	98(3)
C(49)	11054(5)	544(5)	914(4)	69(2)
C(50)	11034(4)	1509(4)	1004(3)	53(1)
C(51)	10424(4)	1895(4)	1470(2)	41(1)

C(52)	9103(4)	1337(3)	3265(3)	40(1)
C(53)	8232(5)	1057(4)	3607(3)	57(1)
C(54)	8434(6)	871(5)	4329(4)	75(2)
C(55)	9492(6)	952(5)	4683(4)	73(2)
C(56)	10333(6)	1217(5)	4340(4)	68(2)
C(57)	10151(5)	1423(4)	3638(3)	55(1)
C(58)	6246(6)	8156(5)	90(5)	80(2)
C(59)	5813(8)	8713(9)	2690(6)	96(3)
C(60)	4153(9)	777(9)	3649(6)	83(3)
Cl(7)	5756(2)	8799(2)	3632(2)	103(1)
Cl(4A)	3328(3)	922(4)	4217(3)	177(3)

Table 102. Bond lengths [Å] and angles [°] for $[Ru(dppp)_2(CO)_2(\mu\text{-}F)_3][SiF_5]$ **(71)**.

Ru(1)-C(1)	1.814(4)	Ru(1)-F(3)	2.098(3)
Ru(1)-F(2)	2.112(2)	Ru(1)-F(1)	2.117(2)
Ru(1)-P(2)	2.2736(10)	Ru(1)-P(1)	2.2881(10)
Ru(1)-Ru(2)	3.0164(4)	Ru(2)-C(2)	1.812(4)
Ru(2)-F(3)	2.115(2)	Ru(2)-F(1)	2.116(2)
Ru(2)-F(2)	2.130(2)	Ru(2)-P(4)	2.2614(10)
Ru(2)-P(3)	2.2891(10)	Cl(2)-C(59)	1.684(12)
Cl(3)-C(60)	1.673(12)	Cl(5)-C(58)	1.763(6)
Cl(6)-C(58)	1.742(7)	P(1)-C(9)	1.825(4)
P(1)-C(15)	1.826(4)	P(1)-C(3)	1.833(5)
P(2)-C(21)	1.816(4)	P(2)-C(5)	1.829(4)
P(2)-C(27)	1.836(4)	P(3)-C(40)	1.818(4)
P(3)-C(6)	1.829(4)	P(3)-C(34)	1.833(4)
P(4)-C(52)	1.821(4)	P(4)-C(46)	1.820(4)
P(4)-C(8)	1.828(4)	Si(1)-F(38)	1.544(6)
Si(1)-F(91)	1.549(4)	Si(1)-F(4)	1.568(5)
Si(1)-F(52)	1.567(4)	Si(1)-F(71)	1.599(6)
O(2)-C(2)	1.153(5)	O(90)-C(1)	1.157(5)
C(3)-C(4)	1.523(7)	C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900	C(4)-C(5)	1.536(6)
C(4)-H(4A)	0.9900	C(4)-H(4B)	0.9900
C(5)-H(5A)	0.9900	C(5)-H(5B)	0.9900
C(6)-C(7)	1.546(6)	C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900	C(7)-C(8)	1.531(6)
C(7)-H(7A)	0.9900	C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900	C(8)-H(8B)	0.9900
C(9)-C(10)	1.375(6)	C(9)-C(14)	1.393(6)
C(10)-C(11)	1.393(6)	C(10)-H(10)	0.9500
C(11)-C(12)	1.394(7)	C(11)-H(11)	0.9500
C(12)-C(13)	1.379(8)	C(12)-H(12)	0.9500
C(13)-C(14)	1.393(7)	C(13)-H(13)	0.9500
C(14)-H(14)	0.9500	C(15)-C(20)	1.377(7)
C(15)-C(16)	1.383(7)	C(16)-C(17)	1.373(7)
C(16)-H(16)	0.9500	C(17)-C(18)	1.380(9)
C(17)-H(17)	0.9500	C(18)-C(19)	1.386(12)
C(18)-H(18)	0.9500	C(19)-C(20)	1.396(10)
C(19)-H(19)	0.9500	C(20)-H(20)	0.9500
C(21)-C(22)	1.388(6)	C(21)-C(26)	1.401(6)
C(22)-C(23)	1.393(6)	C(22)-H(22)	0.9500
C(23)-C(24)	1.388(7)	C(23)-H(23)	0.9500
C(24)-C(25)	1.368(8)	C(24)-H(24)	0.9500

C(25)-C(26)	1.389(7)	C(26)-H(26)	0.9500
C(27)-C(32)	1.386(6)	C(27)-C(28)	1.390(6)
C(28)-C(29)	1.387(7)	C(28)-H(28)	0.9500
C(29)-C(30)	1.375(7)	C(29)-H(29)	0.9500
C(30)-C(31)	1.375(7)	C(30)-H(30)	0.9500
C(31)-C(32)	1.389(6)	C(31)-H(31)	0.9500
C(32)-H(32)	0.9500	C(34)-C(35)	1.387(6)
C(34)-C(39)	1.388(6)	C(35)-C(36)	1.390(6)
C(35)-H(35)	0.9500	C(36)-C(37)	1.380(7)
C(36)-H(36)	0.9500	C(37)-C(38)	1.378(7)
C(37)-H(37)	0.9500	C(38)-C(39)	1.394(6)
C(38)-H(38)	0.9500	C(39)-H(39)	0.9500
C(40)-C(45)	1.394(6)	C(40)-C(41)	1.393(6)
C(41)-C(42)	1.396(6)	C(41)-H(41)	0.9500
C(42)-C(43)	1.357(8)	C(42)-H(42)	0.9500
C(43)-C(44)	1.392(8)	C(43)-H(43)	0.9500
C(44)-C(45)	1.383(6)	C(44)-H(44)	0.9500
C(45)-H(45)	0.9500	C(46)-C(47)	1.384(7)
C(46)-C(51)	1.385(7)	C(47)-C(48)	1.381(9)
C(47)-H(47)	0.9500	C(48)-C(49)	1.370(10)
C(48)-H(48)	0.9500	C(49)-C(50)	1.368(8)
C(49)-H(49)	0.9500	C(50)-C(51)	1.389(6)
C(50)-H(50)	0.9500	C(51)-H(51)	0.9500
C(52)-C(57)	1.384(7)	C(52)-C(53)	1.387(7)
C(53)-C(54)	1.409(8)	C(53)-H(53)	0.9500
C(54)-C(55)	1.387(10)	C(54)-H(54)	0.9500
C(55)-C(56)	1.353(10)	C(55)-H(55)	0.9500
C(56)-C(57)	1.385(8)	C(56)-H(56)	0.9500
C(57)-H(57)	0.9500	C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900	C(59)-Cl(7)	1.732(10)
C(59)-H(59A)	0.9900	C(59)-H(59B)	0.9900
C(60)-Cl(4A)	1.635(10)	C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900		
C(1)-Ru(1)-F(3)	101.58(15)	C(1)-Ru(1)-F(2)	169.80(15)
F(3)-Ru(1)-F(2)	73.34(9)	C(1)-Ru(1)-F(1)	96.89(15)
F(3)-Ru(1)-F(1)	77.86(9)	F(2)-Ru(1)-F(1)	73.53(8)
C(1)-Ru(1)-P(2)	87.98(14)	F(3)-Ru(1)-P(2)	92.90(8)
F(2)-Ru(1)-P(2)	100.98(6)	F(1)-Ru(1)-P(2)	170.23(7)
C(1)-Ru(1)-P(1)	85.52(14)	F(3)-Ru(1)-P(1)	171.00(7)
F(2)-Ru(1)-P(1)	98.76(6)	F(1)-Ru(1)-P(1)	95.95(7)
P(2)-Ru(1)-P(1)	92.86(4)	C(1)-Ru(1)-Ru(2)	125.42(14)
F(3)-Ru(1)-Ru(2)	44.51(7)	F(2)-Ru(1)-Ru(2)	44.92(6)
F(1)-Ru(1)-Ru(2)	44.54(6)	P(2)-Ru(1)-Ru(2)	126.00(3)
P(1)-Ru(1)-Ru(2)	126.68(3)	C(2)-Ru(2)-F(3)	97.19(14)
C(2)-Ru(2)-F(1)	98.47(14)	F(3)-Ru(2)-F(1)	77.50(9)
C(2)-Ru(2)-F(2)	167.83(14)	F(3)-Ru(2)-F(2)	72.63(9)
F(1)-Ru(2)-F(2)	73.17(8)	C(2)-Ru(2)-P(4)	86.24(13)
F(3)-Ru(2)-P(4)	94.97(8)	F(1)-Ru(2)-P(4)	171.51(7)
F(2)-Ru(2)-P(4)	101.02(6)	C(2)-Ru(2)-P(3)	89.37(13)
F(3)-Ru(2)-P(3)	171.02(7)	F(1)-Ru(2)-P(3)	95.53(7)
F(2)-Ru(2)-P(3)	100.09(6)	P(4)-Ru(2)-P(3)	91.56(4)
C(2)-Ru(2)-Ru(1)	123.46(13)	F(3)-Ru(2)-Ru(1)	44.05(7)
F(1)-Ru(2)-Ru(1)	44.56(6)	F(2)-Ru(2)-Ru(1)	44.44(6)
P(4)-Ru(2)-Ru(1)	127.01(3)	P(3)-Ru(2)-Ru(1)	127.00(3)

C(9)-P(1)-C(15)	104.0(2)	C(9)-P(1)-C(3)	102.4(2)
C(15)-P(1)-C(3)	104.7(2)	C(9)-P(1)-Ru(1)	118.18(14)
C(15)-P(1)-Ru(1)	112.60(15)	C(3)-P(1)-Ru(1)	113.48(16)
C(21)-P(2)-C(5)	105.5(2)	C(21)-P(2)-C(27)	102.46(19)
C(5)-P(2)-C(27)	103.3(2)	C(21)-P(2)-Ru(1)	116.50(13)
C(5)-P(2)-Ru(1)	113.92(16)	C(27)-P(2)-Ru(1)	113.65(14)
C(40)-P(3)-C(6)	106.1(2)	C(40)-P(3)-C(34)	102.50(18)
C(6)-P(3)-C(34)	102.62(19)	C(40)-P(3)-Ru(2)	115.25(13)
C(6)-P(3)-Ru(2)	114.86(14)	C(34)-P(3)-Ru(2)	113.99(13)
C(52)-P(4)-C(46)	105.7(2)	C(52)-P(4)-C(8)	105.4(2)
C(46)-P(4)-C(8)	102.7(2)	C(52)-P(4)-Ru(2)	109.57(14)
C(46)-P(4)-Ru(2)	117.74(15)	C(8)-P(4)-Ru(2)	114.67(15)
F(38)-Si(1)-F(91)	122.8(3)	F(38)-Si(1)-F(4)	89.3(4)
F(91)-Si(1)-F(4)	92.4(3)	F(38)-Si(1)-F(52)	122.7(3)
F(91)-Si(1)-F(52)	114.0(3)	F(4)-Si(1)-F(52)	94.9(3)
F(38)-Si(1)-F(71)	79.8(4)	F(91)-Si(1)-F(71)	92.2(3)
F(4)-Si(1)-F(71)	168.9(4)	F(52)-Si(1)-F(71)	92.4(3)
Ru(1)-F(1)-Ru(2)	90.91(8)	Ru(1)-F(2)-Ru(2)	90.64(8)
Ru(1)-F(3)-Ru(2)	91.45(10)	O(90)-C(1)-Ru(1)	177.9(4)
O(2)-C(2)-Ru(2)	177.1(4)	C(4)-C(3)-P(1)	114.6(3)
C(4)-C(3)-H(3A)	108.6	P(1)-C(3)-H(3A)	108.6
C(4)-C(3)-H(3B)	108.6	P(1)-C(3)-H(3B)	108.6
H(3A)-C(3)-H(3B)	107.6	C(3)-C(4)-C(5)	115.4(4)
C(3)-C(4)-H(4A)	108.4	C(5)-C(4)-H(4A)	108.4
C(3)-C(4)-H(4B)	108.4	C(5)-C(4)-H(4B)	108.4
H(4A)-C(4)-H(4B)	107.5	C(4)-C(5)-P(2)	114.6(3)
C(4)-C(5)-H(5A)	108.6	P(2)-C(5)-H(5A)	108.6
C(4)-C(5)-H(5B)	108.6	P(2)-C(5)-H(5B)	108.6
H(5A)-C(5)-H(5B)	107.6	C(7)-C(6)-P(3)	115.4(3)
C(7)-C(6)-H(6A)	108.4	P(3)-C(6)-H(6A)	108.4
C(7)-C(6)-H(6B)	108.4	P(3)-C(6)-H(6B)	108.4
H(6A)-C(6)-H(6B)	107.5	C(8)-C(7)-C(6)	114.8(4)
C(8)-C(7)-H(7A)	108.6	C(6)-C(7)-H(7A)	108.6
C(8)-C(7)-H(7B)	108.6	C(6)-C(7)-H(7B)	108.6
H(7A)-C(7)-H(7B)	107.5	C(7)-C(8)-P(4)	113.3(3)
C(7)-C(8)-H(8A)	108.9	P(4)-C(8)-H(8A)	108.9
C(7)-C(8)-H(8B)	108.9	P(4)-C(8)-H(8B)	108.9
H(8A)-C(8)-H(8B)	107.7	C(10)-C(9)-C(14)	119.4(4)
C(10)-C(9)-P(1)	120.6(3)	C(14)-C(9)-P(1)	119.9(3)
C(9)-C(10)-C(11)	120.9(4)	C(9)-C(10)-H(10)	119.5
C(11)-C(10)-H(10)	119.5	C(12)-C(11)-C(10)	119.1(5)
C(12)-C(11)-H(11)	120.4	C(10)-C(11)-H(11)	120.4
C(13)-C(12)-C(11)	120.5(4)	C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8	C(12)-C(13)-C(14)	119.6(5)
C(12)-C(13)-H(13)	120.2	C(14)-C(13)-H(13)	120.2
C(13)-C(14)-C(9)	120.4(5)	C(13)-C(14)-H(14)	119.8
C(9)-C(14)-H(14)	119.8	C(20)-C(15)-C(16)	118.9(5)
C(20)-C(15)-P(1)	122.5(4)	C(16)-C(15)-P(1)	118.6(3)
C(17)-C(16)-C(15)	121.5(5)	C(17)-C(16)-H(16)	119.3
C(15)-C(16)-H(16)	119.3	C(16)-C(17)-C(18)	120.0(6)
C(16)-C(17)-H(17)	120.0	C(18)-C(17)-H(17)	120.0
C(17)-C(18)-C(19)	119.3(6)	C(17)-C(18)-H(18)	120.3
C(19)-C(18)-H(18)	120.3	C(18)-C(19)-C(20)	120.2(7)
C(18)-C(19)-H(19)	119.9	C(20)-C(19)-H(19)	119.9
C(15)-C(20)-C(19)	120.1(7)	C(15)-C(20)-H(20)	119.9

C(19)-C(20)-H(20)	119.9	C(22)-C(21)-C(26)	119.0(4)
C(22)-C(21)-P(2)	118.5(3)	C(26)-C(21)-P(2)	122.4(3)
C(21)-C(22)-C(23)	120.0(4)	C(21)-C(22)-H(22)	120.0
C(23)-C(22)-H(22)	120.0	C(24)-C(23)-C(22)	120.0(5)
C(24)-C(23)-H(23)	120.0	C(22)-C(23)-H(23)	120.0
C(25)-C(24)-C(23)	120.6(4)	C(25)-C(24)-H(24)	119.7
C(23)-C(24)-H(24)	119.7	C(24)-C(25)-C(26)	119.8(4)
C(25)-C(26)-C(21)	120.6(4)	C(25)-C(26)-H(26)	119.7
C(21)-C(26)-H(26)	119.7	C(32)-C(27)-C(28)	118.6(4)
C(32)-C(27)-P(2)	121.0(3)	C(28)-C(27)-P(2)	120.4(3)
C(29)-C(28)-C(27)	120.6(4)	C(29)-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7	C(30)-C(29)-C(28)	120.1(5)
C(30)-C(29)-H(29)	120.0	C(28)-C(29)-H(29)	120.0
C(31)-C(30)-C(29)	119.9(4)	C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0	C(30)-C(31)-C(32)	120.2(4)
C(30)-C(31)-H(31)	119.9	C(32)-C(31)-H(31)	119.9
C(27)-C(32)-C(31)	120.6(4)	C(27)-C(32)-H(32)	119.7
C(31)-C(32)-H(32)	119.7	C(35)-C(34)-C(39)	118.3(4)
C(35)-C(34)-P(3)	121.3(3)	C(39)-C(34)-P(3)	120.3(3)
C(34)-C(35)-C(36)	121.0(4)	C(34)-C(35)-H(35)	119.5
C(36)-C(35)-H(35)	119.5	C(37)-C(36)-C(35)	119.9(4)
C(37)-C(36)-H(36)	120.0	C(35)-C(36)-H(36)	120.0
C(38)-C(37)-C(36)	120.1(4)	C(38)-C(37)-H(37)	120.0
C(36)-C(37)-H(37)	120.0	C(37)-C(38)-C(39)	119.8(4)
C(37)-C(38)-H(38)	120.1	C(39)-C(38)-H(38)	120.1
C(34)-C(39)-C(38)	120.9(4)	C(34)-C(39)-H(39)	119.5
C(38)-C(39)-H(39)	119.5	C(45)-C(40)-C(41)	118.9(4)
C(45)-C(40)-P(3)	118.0(3)	C(41)-C(40)-P(3)	123.1(3)
C(40)-C(41)-C(42)	119.9(5)	C(40)-C(41)-H(41)	120.1
C(42)-C(41)-H(41)	120.1	C(43)-C(42)-C(41)	120.7(5)
C(43)-C(42)-H(42)	119.7	C(41)-C(42)-H(42)	119.7
C(42)-C(43)-C(44)	120.2(4)	C(42)-C(43)-H(43)	119.9
C(44)-C(43)-H(43)	119.9	C(45)-C(44)-C(43)	119.8(5)
C(45)-C(44)-H(44)	120.1	C(43)-C(44)-H(44)	120.1
C(44)-C(45)-C(40)	120.6(4)	C(44)-C(45)-H(45)	119.7
C(40)-C(45)-H(45)	119.7	C(47)-C(46)-C(51)	118.9(5)
C(47)-C(46)-P(4)	119.9(4)	C(51)-C(46)-P(4)	120.9(3)
C(48)-C(47)-C(46)	120.2(6)	C(48)-C(47)-H(47)	119.9
C(46)-C(47)-H(47)	119.9	C(49)-C(48)-C(47)	121.0(6)
C(49)-C(48)-H(48)	119.5	C(47)-C(48)-H(48)	119.5
C(50)-C(49)-C(48)	118.8(5)	C(50)-C(49)-H(49)	120.6
C(48)-C(49)-H(49)	120.6	C(49)-C(50)-C(51)	121.3(5)
C(49)-C(50)-H(50)	119.3	C(51)-C(50)-H(50)	119.3
C(46)-C(51)-C(50)	119.6(5)	C(46)-C(51)-H(51)	120.2
C(50)-C(51)-H(51)	120.2	C(57)-C(52)-C(53)	119.3(5)
C(57)-C(52)-P(4)	120.0(4)	C(53)-C(52)-P(4)	120.3(4)
C(52)-C(53)-C(54)	119.3(5)	C(52)-C(53)-H(53)	120.4
C(54)-C(53)-H(53)	120.4	C(55)-C(54)-C(53)	119.9(6)
C(55)-C(54)-H(54)	120.0	C(53)-C(54)-H(54)	120.0
C(56)-C(55)-C(54)	120.2(5)	C(56)-C(55)-H(55)	119.9
C(54)-C(55)-H(55)	119.9	C(55)-C(56)-C(57)	120.6(6)
C(55)-C(56)-H(56)	119.7	C(57)-C(56)-H(56)	119.7
C(52)-C(57)-C(56)	120.7(6)	C(52)-C(57)-H(57)	119.6
C(56)-C(57)-H(57)	119.6	Cl(6)-C(58)-Cl(5)	111.5(4)
Cl(6)-C(58)-H(58A)	109.3	Cl(5)-C(58)-H(58A)	109.3

Cl(6)-C(58)-H(58B)	109.3	Cl(5)-C(58)-H(58B)	109.3
H(58A)-C(58)-H(58B)	108.0	Cl(2)-C(59)-Cl(7)	116.8(6)
Cl(2)-C(59)-H(59A)	108.1	Cl(7)-C(59)-H(59A)	108.1
Cl(2)-C(59)-H(59B)	108.1	Cl(7)-C(59)-H(59B)	108.1
H(59A)-C(59)-H(59B)	107.3	Cl(4A)-C(60)-Cl(3)	116.9(6)
Cl(4A)-C(60)-H(60A)	108.1	Cl(3)-C(60)-H(60A)	108.1
Cl(4A)-C(60)-H(60B)	108.1	Cl(3)-C(60)-H(60B)	108.1
H(60A)-C(60)-H(60B)	107.3		

Table 103. Anisotropic displacement parameters ($Å^2$ x 10^3) for $[Ru(dppp)_2(CO)_2(\mu\text{-}F)_3][SiF_5]$ **(71)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	28(1)	28(1)	27(1)	8(1)	8(1)	8(1)
Ru(2)	25(1)	28(1)	28(1)	11(1)	9(1)	9(1)
Cl(2)	225(4)	89(2)	188(4)	35(2)	121(3)	84(3)
Cl(3)	118(3)	129(3)	159(4)	-39(3)	68(3)	-11(2)
Cl(5)	62(1)	59(1)	119(1)	24(1)	-6(1)	13(1)
Cl(6)	71(1)	122(2)	72(1)	5(1)	16(1)	-1(1)
P(1)	37(1)	28(1)	34(1)	10(1)	10(1)	7(1)
P(2)	28(1)	35(1)	30(1)	9(1)	7(1)	8(1)
P(3)	27(1)	32(1)	30(1)	11(1)	8(1)	11(1)
P(4)	33(1)	28(1)	36(1)	12(1)	9(1)	10(1)
Si(1)	50(1)	48(1)	55(1)	15(1)	11(1)	16(1)
F(1)	34(1)	34(1)	37(1)	13(1)	9(1)	13(1)
F(2)	28(1)	31(1)	28(1)	9(1)	9(1)	10(1)
F(3)	43(1)	43(1)	41(1)	15(1)	7(1)	7(1)
F(4)	106(4)	190(6)	83(3)	3(3)	-9(3)	50(4)
F(38)	208(7)	69(3)	177(6)	19(3)	91(5)	22(4)
F(52)	139(4)	97(3)	144(4)	48(3)	95(4)	75(3)
F(71)	73(3)	271(9)	110(4)	2(5)	7(3)	43(4)
F(91)	121(4)	89(3)	121(4)	38(3)	66(3)	11(3)
O(2)	38(2)	54(2)	58(2)	25(2)	26(2)	16(1)
O(90)	65(2)	47(2)	36(2)	4(1)	18(2)	20(2)
C(1)	38(2)	39(2)	37(2)	12(2)	11(2)	14(2)
C(2)	32(2)	38(2)	36(2)	16(2)	8(2)	14(2)
C(3)	45(2)	33(2)	44(2)	5(2)	12(2)	0(2)
C(4)	37(2)	38(2)	44(2)	7(2)	5(2)	-4(2)
C(5)	36(2)	47(2)	33(2)	7(2)	5(2)	5(2)
C(6)	32(2)	37(2)	37(2)	11(2)	3(2)	8(2)
C(7)	41(2)	32(2)	45(2)	10(2)	1(2)	7(2)
C(8)	38(2)	32(2)	48(2)	12(2)	6(2)	4(2)
C(9)	32(2)	40(2)	33(2)	10(2)	9(2)	7(2)
C(10)	38(2)	46(2)	39(2)	16(2)	13(2)	14(2)
C(11)	45(3)	62(3)	45(2)	15(2)	16(2)	22(2)
C(12)	35(2)	71(3)	35(2)	15(2)	11(2)	11(2)
C(13)	51(3)	61(3)	44(3)	23(2)	19(2)	6(2)
C(14)	49(3)	44(2)	47(2)	18(2)	18(2)	11(2)
C(15)	59(3)	34(2)	44(2)	20(2)	24(2)	21(2)
C(16)	51(3)	41(3)	66(3)	18(2)	15(2)	20(2)
C(17)	61(3)	65(3)	75(4)	41(3)	27(3)	37(3)
C(18)	121(6)	87(5)	74(4)	48(4)	38(4)	74(5)
C(19)	202(10)	69(5)	78(5)	19(4)	28(6)	90(6)

C(20)	121(6)	43(3)	69(4)	11(3)	-1(4)	37(3)
C(21)	30(2)	43(2)	33(2)	14(2)	10(2)	14(2)
C(22)	34(2)	44(2)	40(2)	9(2)	3(2)	18(2)
C(23)	49(3)	58(3)	43(2)	1(2)	3(2)	29(2)
C(24)	51(3)	72(4)	47(3)	9(2)	16(2)	34(3)
C(25)	38(2)	69(3)	51(3)	18(2)	17(2)	22(2)
C(26)	30(2)	52(3)	38(2)	16(2)	10(2)	13(2)
C(27)	32(2)	42(2)	30(2)	11(2)	4(2)	8(2)
C(28)	63(3)	62(3)	42(2)	22(2)	21(2)	35(3)
C(29)	79(4)	83(4)	42(3)	31(3)	32(3)	47(3)
C(30)	60(3)	63(3)	40(2)	27(2)	17(2)	24(2)
C(31)	49(3)	50(3)	52(3)	22(2)	10(2)	21(2)
C(32)	34(2)	49(3)	47(2)	18(2)	14(2)	17(2)
C(34)	30(2)	35(2)	34(2)	10(2)	6(2)	14(2)
C(35)	45(2)	42(2)	40(2)	15(2)	16(2)	22(2)
C(36)	50(3)	47(3)	44(2)	22(2)	12(2)	25(2)
C(37)	40(2)	41(2)	53(3)	16(2)	9(2)	22(2)
C(38)	59(3)	71(3)	48(3)	21(2)	26(2)	44(3)
C(39)	52(3)	64(3)	43(2)	27(2)	23(2)	37(2)
C(40)	35(2)	38(2)	32(2)	16(2)	13(2)	19(2)
C(41)	50(3)	46(2)	39(2)	15(2)	17(2)	23(2)
C(42)	68(3)	58(3)	43(2)	18(2)	26(2)	36(3)
C(43)	59(3)	80(4)	50(3)	32(3)	31(2)	38(3)
C(44)	39(2)	68(3)	51(3)	33(2)	21(2)	22(2)
C(45)	36(2)	49(2)	35(2)	21(2)	11(2)	16(2)
C(46)	41(2)	36(2)	44(2)	4(2)	9(2)	16(2)
C(47)	93(5)	41(3)	111(5)	26(3)	52(4)	32(3)
C(48)	122(7)	54(4)	138(7)	8(4)	61(6)	53(4)
C(49)	63(3)	68(4)	73(4)	-11(3)	24(3)	32(3)
C(50)	42(2)	77(4)	43(3)	7(2)	13(2)	28(2)
C(51)	41(2)	49(3)	37(2)	10(2)	10(2)	23(2)
C(52)	50(3)	31(2)	46(2)	17(2)	14(2)	16(2)
C(53)	64(3)	61(3)	58(3)	30(3)	20(3)	24(3)
C(54)	90(5)	91(5)	71(4)	51(4)	40(4)	39(4)
C(55)	111(5)	69(4)	57(3)	36(3)	17(4)	44(4)
C(56)	77(4)	63(4)	67(4)	32(3)	-2(3)	26(3)
C(57)	55(3)	49(3)	61(3)	29(2)	1(2)	13(2)
C(58)	76(4)	46(3)	119(6)	19(3)	31(4)	19(3)
C(59)	82(6)	113(8)	82(6)	38(6)	7(5)	11(6)
C(60)	93(7)	99(8)	62(5)	12(5)	30(5)	39(6)
Cl(7)	83(2)	134(2)	123(2)	86(2)	45(2)	30(2)
Cl(4A)	95(2)	182(4)	170(4)	-98(3)	65(2)	-7(2)

Table 104. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for $[Ru(dppp)_2(CO)_2(\mu\text{-}F)_3][SiF_5]$ **(71)**.

Atom	x	y	z	U(eq)
H(3A)	13520	7868	3777	53
H(3B)	12911	7572	4423	53
H(4A)	14715	7370	4528	53
H(4B)	14226	6471	3776	53
H(5A)	13436	6415	5134	50
H(5B)	14384	5950	4947	50
H(6A)	6409	2134	1374	43

H(6B)	6650	2094	548	43
H(7A)	6586	548	747	50
H(7B)	7849	1105	800	50
H(8A)	7523	212	1768	49
H(8B)	6985	1027	2127	49
H(10)	12630	4852	2410	47
H(11)	13597	4685	1446	58
H(12)	14068	5987	852	57
H(13)	13535	7412	1194	62
H(14)	12636	7596	2194	55
H(16)	9968	6092	2223	61
H(17)	8776	6985	1954	70
H(18)	9164	8643	2643	95
H(19)	10832	9428	3534	128
H(20)	12038	8517	3798	94
H(22)	11983	3113	3006	47
H(23)	12850	2157	2281	60
H(24)	14751	2718	2426	65
H(26)	14949	5165	4034	47
H(28)	11527	4908	5412	60
H(29)	11360	4068	6364	71
H(30)	12202	2836	6430	61
H(31)	13280	2492	5580	58
H(32)	13451	3326	4624	49
H(35)	7773	4369	371	47
H(36)	6916	5593	280	52
H(37)	6118	6175	1252	51
H(38)	6190	5547	2321	63
H(39)	7097	4357	2428	55
H(41)	7962	2107	-93	50
H(42)	9055	2306	-980	61
H(43)	10697	3573	-666	66
H(44)	11260	4717	531	58
H(45)	10192	4531	1426	45
H(47)	9456	-94	2035	90
H(48)	10452	-722	1226	118
H(49)	11476	289	595	83
H(50)	11445	1923	742	63
H(51)	10425	2569	1530	49
H(53)	7507	992	3358	68
H(54)	7846	690	4572	90
H(55)	9627	822	5167	87
H(56)	11054	1263	4582	81
H(57)	10752	1626	3410	66
H(58A)	6332	8526	-306	96
H(58B)	5873	8482	446	96
H(59A)	5087	8289	2369	115
H(59B)	5936	9391	2607	115
H(60A)	3936	1026	3205	99
H(60B)	4036	51	3461	99

Table 105. Dihedral angles [°] for $[Ru(dppp)_2(CO)_2(\mu\text{-}F)_3][SiF_5]$ **(71)**.

Atom1 - Atom2 - Atom3 - Atom4	Dihedral
C(1) - Ru(1) - Ru(2) - C(2)	-6.0(2)
F(3) - Ru(1) - Ru(2) - C(2)	62.12(18)
F(2) - Ru(1) - Ru(2) - C(2)	178.29(17)
F(1) - Ru(1) - Ru(2) - C(2)	-65.19(17)
P(2) - Ru(1) - Ru(2) - C(2)	111.57(15)
P(1) - Ru(1) - Ru(2) - C(2)	-120.26(15)
C(1) - Ru(1) - Ru(2) - F(3)	-68.16(19)
F(2) - Ru(1) - Ru(2) - F(3)	116.17(13)
F(1) - Ru(1) - Ru(2) - F(3)	-127.31(14)
P(2) - Ru(1) - Ru(2) - F(3)	49.45(11)
P(1) - Ru(1) - Ru(2) - F(3)	177.62(11)
C(1) - Ru(1) - Ru(2) - F(1)	59.15(18)
F(3) - Ru(1) - Ru(2) - F(1)	127.31(14)
F(2) - Ru(1) - Ru(2) - F(1)	-116.52(12)
P(2) - Ru(1) - Ru(2) - F(1)	176.76(9)
P(1) - Ru(1) - Ru(2) - F(1)	-55.07(9)
C(1) - Ru(1) - Ru(2) - F(2)	175.67(18)
F(3) - Ru(1) - Ru(2) - F(2)	-116.17(13)
F(1) - Ru(1) - Ru(2) - F(2)	116.52(12)
P(2) - Ru(1) - Ru(2) - F(2)	-66.72(9)
P(1) - Ru(1) - Ru(2) - F(2)	61.45(9)
C(1) - Ru(1) - Ru(2) - P(4)	-119.60(17)
F(3) - Ru(1) - Ru(2) - P(4)	-51.44(11)
F(2) - Ru(1) - Ru(2) - P(4)	64.73(9)
F(1) - Ru(1) - Ru(2) - P(4)	-178.75(9)
P(2) - Ru(1) - Ru(2) - P(4)	-1.99(5)
P(1) - Ru(1) - Ru(2) - P(4)	126.18(5)
C(1) - Ru(1) - Ru(2) - P(3)	112.75(16)
F(3) - Ru(1) - Ru(2) - P(3)	-179.09(11)
F(2) - Ru(1) - Ru(2) - P(3)	-62.92(9)
F(1) - Ru(1) - Ru(2) - P(3)	53.60(9)
P(2) - Ru(1) - Ru(2) - P(3)	-129.64(5)
P(1) - Ru(1) - Ru(2) - P(3)	-1.47(5)
C(1) - Ru(1) - P(1) - C(9)	168.2(2)
F(3) - Ru(1) - P(1) - C(9)	-49.2(5)
F(2) - Ru(1) - P(1) - C(9)	-21.08(17)
F(1) - Ru(1) - P(1) - C(9)	-95.27(17)
P(2) - Ru(1) - P(1) - C(9)	80.50(16)
Ru(2) - Ru(1) - P(1) - C(9)	-59.95(16)
C(1) - Ru(1) - P(1) - C(15)	-70.4(2)
F(3) - Ru(1) - P(1) - C(15)	72.1(5)
F(2) - Ru(1) - P(1) - C(15)	100.24(17)
F(1) - Ru(1) - P(1) - C(15)	26.05(18)
P(2) - Ru(1) - P(1) - C(15)	-158.18(17)
Ru(2) - Ru(1) - P(1) - C(15)	61.37(17)
C(1) - Ru(1) - P(1) - C(3)	48.3(2)
F(3) - Ru(1) - P(1) - C(3)	-169.1(5)
F(2) - Ru(1) - P(1) - C(3)	-140.99(18)
F(1) - Ru(1) - P(1) - C(3)	144.82(18)
P(2) - Ru(1) - P(1) - C(3)	-39.42(18)
Ru(2) - Ru(1) - P(1) - C(3)	-179.86(17)

C(1) - Ru(1) - P(2) - C(21)	-169.2(2)
F(3) - Ru(1) - P(2) - C(21)	89.29(17)
F(2) - Ru(1) - P(2) - C(21)	15.70(17)
F(1) - Ru(1) - P(2) - C(21)	70.6(4)
P(1) - Ru(1) - P(2) - C(21)	-83.79(16)
Ru(2) - Ru(1) - P(2) - C(21)	57.06(16)
C(1) - Ru(1) - P(2) - C(5)	-46.0(2)
F(3) - Ru(1) - P(2) - C(5)	-147.50(17)
F(2) - Ru(1) - P(2) - C(5)	138.92(17)
F(1) - Ru(1) - P(2) - C(5)	-166.2(4)
P(1) - Ru(1) - P(2) - C(5)	39.42(16)
Ru(2) - Ru(1) - P(2) - C(5)	-179.73(15)
C(1) - Ru(1) - P(2) - C(27)	72.0(2)
F(3) - Ru(1) - P(2) - C(27)	-29.49(17)
F(2) - Ru(1) - P(2) - C(27)	-103.08(16)
F(1) - Ru(1) - P(2) - C(27)	-48.2(4)
P(1) - Ru(1) - P(2) - C(27)	157.43(15)
Ru(2) - Ru(1) - P(2) - C(27)	-61.72(16)
C(2) - Ru(2) - P(3) - C(40)	-171.3(2)
F(3) - Ru(2) - P(3) - C(40)	51.6(5)
F(1) - Ru(2) - P(3) - C(40)	90.23(16)
F(2) - Ru(2) - P(3) - C(40)	16.38(16)
P(4) - Ru(2) - P(3) - C(40)	-85.10(15)
Ru(1) - Ru(2) - P(3) - C(40)	55.67(15)
C(2) - Ru(2) - P(3) - C(6)	-47.5(2)
F(3) - Ru(2) - P(3) - C(6)	175.4(5)
F(1) - Ru(2) - P(3) - C(6)	-145.95(17)
F(2) - Ru(2) - P(3) - C(6)	140.20(17)
P(4) - Ru(2) - P(3) - C(6)	38.72(16)
Ru(1) - Ru(2) - P(3) - C(6)	179.49(15)
C(2) - Ru(2) - P(3) - C(34)	70.5(2)
F(3) - Ru(2) - P(3) - C(34)	-66.6(5)
F(1) - Ru(2) - P(3) - C(34)	-27.93(16)
F(2) - Ru(2) - P(3) - C(34)	-101.77(16)
P(4) - Ru(2) - P(3) - C(34)	156.75(15)
Ru(1) - Ru(2) - P(3) - C(34)	-62.49(15)
C(2) - Ru(2) - P(4) - C(52)	-70.7(2)
F(3) - Ru(2) - P(4) - C(52)	26.17(18)
F(1) - Ru(2) - P(4) - C(52)	53.3(5)
F(2) - Ru(2) - P(4) - C(52)	99.41(17)
P(3) - Ru(2) - P(4) - C(52)	-160.00(16)
Ru(1) - Ru(2) - P(4) - C(52)	59.25(17)
C(2) - Ru(2) - P(4) - C(46)	168.5(2)
F(3) - Ru(2) - P(4) - C(46)	-94.57(18)
F(1) - Ru(2) - P(4) - C(46)	-67.4(5)
F(2) - Ru(2) - P(4) - C(46)	-21.33(18)
P(3) - Ru(2) - P(4) - C(46)	79.26(17)
Ru(1) - Ru(2) - P(4) - C(46)	-61.50(17)
C(2) - Ru(2) - P(4) - C(8)	47.6(2)
F(3) - Ru(2) - P(4) - C(8)	144.47(18)
F(1) - Ru(2) - P(4) - C(8)	171.6(5)
F(2) - Ru(2) - P(4) - C(8)	-142.29(18)
P(3) - Ru(2) - P(4) - C(8)	-41.70(17)
Ru(1) - Ru(2) - P(4) - C(8)	177.54(16)
C(1) - Ru(1) - F(1) - Ru(2)	-135.19(15)

F(3) - Ru(1) - F(1) - Ru(2)	-34.77(9)
F(2) - Ru(1) - F(1) - Ru(2)	41.22(8)
P(2) - Ru(1) - F(1) - Ru(2)	-15.6(4)
P(1) - Ru(1) - F(1) - Ru(2)	138.62(6)
C(2) - Ru(2) - F(1) - Ru(1)	130.04(14)
F(3) - Ru(2) - F(1) - Ru(1)	34.50(9)
F(2) - Ru(2) - F(1) - Ru(1)	-40.88(8)
P(4) - Ru(2) - F(1) - Ru(1)	6.8(5)
P(3) - Ru(2) - F(1) - Ru(1)	-139.77(6)
C(1) - Ru(1) - F(2) - Ru(2)	-20.3(8)
F(3) - Ru(1) - F(2) - Ru(2)	41.05(9)
F(1) - Ru(1) - F(2) - Ru(2)	-40.88(8)
P(2) - Ru(1) - F(2) - Ru(2)	130.80(6)
P(1) - Ru(1) - F(2) - Ru(2)	-134.54(6)
C(2) - Ru(2) - F(2) - Ru(1)	-6.8(7)
F(3) - Ru(2) - F(2) - Ru(1)	-40.83(9)
F(1) - Ru(2) - F(2) - Ru(1)	40.99(8)
P(4) - Ru(2) - F(2) - Ru(1)	-132.63(6)
P(3) - Ru(2) - F(2) - Ru(1)	133.76(6)
C(1) - Ru(1) - F(3) - Ru(2)	129.45(15)
F(2) - Ru(1) - F(3) - Ru(2)	-41.42(8)
F(1) - Ru(1) - F(3) - Ru(2)	34.79(9)
P(2) - Ru(1) - F(3) - Ru(2)	-142.01(8)
P(1) - Ru(1) - F(3) - Ru(2)	-12.3(6)
C(2) - Ru(2) - F(3) - Ru(1)	-131.99(15)
F(1) - Ru(2) - F(3) - Ru(1)	-34.86(9)
F(2) - Ru(2) - F(3) - Ru(1)	41.18(8)
P(4) - Ru(2) - F(3) - Ru(1)	141.18(8)
P(3) - Ru(2) - F(3) - Ru(1)	4.7(6)
F(3) - Ru(1) - C(1) - O(90)	-109(11)
F(2) - Ru(1) - C(1) - O(90)	-50(12)
F(1) - Ru(1) - C(1) - O(90)	-30(11)
P(2) - Ru(1) - C(1) - O(90)	158(11)
P(1) - Ru(1) - C(1) - O(90)	65(11)
Ru(2) - Ru(1) - C(1) - O(90)	-68(11)
F(3) - Ru(2) - C(2) - O(2)	15(7)
F(1) - Ru(2) - C(2) - O(2)	-64(7)
F(2) - Ru(2) - C(2) - O(2)	-18(8)
P(4) - Ru(2) - C(2) - O(2)	109(7)
P(3) - Ru(2) - C(2) - O(2)	-159(7)
Ru(1) - Ru(2) - C(2) - O(2)	-24(7)
C(9) - P(1) - C(3) - C(4)	-70.7(4)
C(15) - P(1) - C(3) - C(4)	-179.0(3)
Ru(1) - P(1) - C(3) - C(4)	57.8(4)
P(1) - C(3) - C(4) - C(5)	-71.5(5)
C(3) - C(4) - C(5) - P(2)	71.1(5)
C(21) - P(2) - C(5) - C(4)	71.6(4)
C(27) - P(2) - C(5) - C(4)	178.8(3)
Ru(1) - P(2) - C(5) - C(4)	-57.4(4)
C(40) - P(3) - C(6) - C(7)	73.6(3)
C(34) - P(3) - C(6) - C(7)	-179.3(3)
Ru(2) - P(3) - C(6) - C(7)	-55.0(4)
P(3) - C(6) - C(7) - C(8)	69.0(5)
C(6) - C(7) - C(8) - P(4)	-71.8(5)
C(52) - P(4) - C(8) - C(7)	-177.7(3)

C(46) - P(4) - C(8) - C(7)	-67.3(4)
Ru(2) - P(4) - C(8) - C(7)	61.7(4)
C(15) - P(1) - C(9) - C(10)	-149.6(4)
C(3) - P(1) - C(9) - C(10)	101.5(4)
Ru(1) - P(1) - C(9) - C(10)	-24.0(4)
C(15) - P(1) - C(9) - C(14)	35.6(4)
C(3) - P(1) - C(9) - C(14)	-73.3(4)
Ru(1) - P(1) - C(9) - C(14)	161.2(3)
C(14) - C(9) - C(10) - C(11)	2.7(7)
P(1) - C(9) - C(10) - C(11)	-172.2(4)
C(9) - C(10) - C(11) - C(12)	-1.6(7)
C(10) - C(11) - C(12) - C(13)	-1.0(7)
C(11) - C(12) - C(13) - C(14)	2.4(8)
C(12) - C(13) - C(14) - C(9)	-1.3(8)
C(10) - C(9) - C(14) - C(13)	-1.2(7)
P(1) - C(9) - C(14) - C(13)	173.7(4)
C(9) - P(1) - C(15) - C(20)	-109.9(5)
C(3) - P(1) - C(15) - C(20)	-2.7(5)
Ru(1) - P(1) - C(15) - C(20)	121.0(5)
C(9) - P(1) - C(15) - C(16)	72.0(4)
C(3) - P(1) - C(15) - C(16)	179.1(4)
Ru(1) - P(1) - C(15) - C(16)	-57.1(4)
C(20) - C(15) - C(16) - C(17)	-0.8(8)
P(1) - C(15) - C(16) - C(17)	177.4(4)
C(15) - C(16) - C(17) - C(18)	-0.9(9)
C(16) - C(17) - C(18) - C(19)	2.5(10)
C(17) - C(18) - C(19) - C(20)	-2.4(12)
C(16) - C(15) - C(20) - C(19)	0.9(10)
P(1) - C(15) - C(20) - C(19)	-177.2(6)
C(18) - C(19) - C(20) - C(15)	0.7(12)
C(5) - P(2) - C(21) - C(22)	-173.0(3)
C(27) - P(2) - C(21) - C(22)	79.2(4)
Ru(1) - P(2) - C(21) - C(22)	-45.5(4)
C(5) - P(2) - C(21) - C(26)	10.3(4)
C(27) - P(2) - C(21) - C(26)	-97.6(4)
Ru(1) - P(2) - C(21) - C(26)	137.7(3)
C(26) - C(21) - C(22) - C(23)	0.8(6)
P(2) - C(21) - C(22) - C(23)	-176.1(4)
C(21) - C(22) - C(23) - C(24)	-0.7(7)
C(22) - C(23) - C(24) - C(25)	0.6(8)
C(23) - C(24) - C(25) - C(26)	-0.5(8)
C(24) - C(25) - C(26) - C(21)	0.5(7)
C(22) - C(21) - C(26) - C(25)	-0.7(6)
P(2) - C(21) - C(26) - C(25)	176.0(4)
C(21) - P(2) - C(27) - C(32)	9.5(4)
C(5) - P(2) - C(27) - C(32)	-100.0(4)
Ru(1) - P(2) - C(27) - C(32)	136.1(3)
C(21) - P(2) - C(27) - C(28)	-172.2(4)
C(5) - P(2) - C(27) - C(28)	78.3(4)
Ru(1) - P(2) - C(27) - C(28)	-45.7(4)
C(32) - C(27) - C(28) - C(29)	0.2(8)
P(2) - C(27) - C(28) - C(29)	-178.1(4)
C(27) - C(28) - C(29) - C(30)	-0.8(9)
C(28) - C(29) - C(30) - C(31)	1.4(9)
C(29) - C(30) - C(31) - C(32)	-1.4(8)

C(28) - C(27) - C(32) - C(31)	-0.3(7)
P(2) - C(27) - C(32) - C(31)	178.0(4)
C(30) - C(31) - C(32) - C(27)	0.9(8)
C(40) - P(3) - C(34) - C(35)	19.1(4)
C(6) - P(3) - C(34) - C(35)	-90.9(4)
Ru(2) - P(3) - C(34) - C(35)	144.3(3)
C(40) - P(3) - C(34) - C(39)	-163.7(4)
C(6) - P(3) - C(34) - C(39)	86.4(4)
Ru(2) - P(3) - C(34) - C(39)	-38.4(4)
C(39) - C(34) - C(35) - C(36)	0.1(7)
P(3) - C(34) - C(35) - C(36)	177.3(4)
C(34) - C(35) - C(36) - C(37)	-0.7(7)
C(35) - C(36) - C(37) - C(38)	0.4(8)
C(36) - C(37) - C(38) - C(39)	0.6(8)
C(35) - C(34) - C(39) - C(38)	1.0(7)
P(3) - C(34) - C(39) - C(38)	-176.3(4)
C(37) - C(38) - C(39) - C(34)	-1.3(8)
C(6) - P(3) - C(40) - C(45)	-176.1(3)
C(34) - P(3) - C(40) - C(45)	76.6(3)
Ru(2) - P(3) - C(40) - C(45)	-47.8(3)
C(6) - P(3) - C(40) - C(41)	5.8(4)
C(34) - P(3) - C(40) - C(41)	-101.4(4)
Ru(2) - P(3) - C(40) - C(41)	134.1(3)
C(45) - C(40) - C(41) - C(42)	-0.3(6)
P(3) - C(40) - C(41) - C(42)	177.8(3)
C(40) - C(41) - C(42) - C(43)	0.6(7)
C(41) - C(42) - C(43) - C(44)	-1.1(8)
C(42) - C(43) - C(44) - C(45)	1.3(7)
C(43) - C(44) - C(45) - C(40)	-1.0(7)
C(41) - C(40) - C(45) - C(44)	0.5(6)
P(3) - C(40) - C(45) - C(44)	-177.7(3)
C(52) - P(4) - C(46) - C(47)	47.3(5)
C(8) - P(4) - C(46) - C(47)	-63.0(5)
Ru(2) - P(4) - C(46) - C(47)	170.0(5)
C(52) - P(4) - C(46) - C(51)	-137.6(4)
C(8) - P(4) - C(46) - C(51)	112.2(4)
Ru(2) - P(4) - C(46) - C(51)	-14.8(4)
C(51) - C(46) - C(47) - C(48)	-2.2(10)
P(4) - C(46) - C(47) - C(48)	173.1(6)
C(46) - C(47) - C(48) - C(49)	2.0(13)
C(47) - C(48) - C(49) - C(50)	-1.0(12)
C(48) - C(49) - C(50) - C(51)	0.3(9)
C(47) - C(46) - C(51) - C(50)	1.5(7)
P(4) - C(46) - C(51) - C(50)	-173.8(4)
C(49) - C(50) - C(51) - C(46)	-0.5(7)
C(46) - P(4) - C(52) - C(57)	41.3(4)
C(8) - P(4) - C(52) - C(57)	149.6(4)
Ru(2) - P(4) - C(52) - C(57)	-86.5(4)
C(46) - P(4) - C(52) - C(53)	-145.9(4)
C(8) - P(4) - C(52) - C(53)	-37.6(5)
Ru(2) - P(4) - C(52) - C(53)	86.3(4)
C(57) - C(52) - C(53) - C(54)	0.2(8)
P(4) - C(52) - C(53) - C(54)	-172.6(5)
C(52) - C(53) - C(54) - C(55)	-1.0(10)
C(53) - C(54) - C(55) - C(56)	0.5(10)

C(54) - C(55) - C(56) - C(57)	0.9(10)
C(53) - C(52) - C(57) - C(56)	1.1(8)
P(4) - C(52) - C(57) - C(56)	174.0(4)
C(55) - C(56) - C(57) - C(52)	-1.7(9)

Table 106. Crystal data and structure refinement for $Ru(IMe_4)(dppp)(CO)HF$ **(76)**.

Compound	$Ru(IMe_4)(dppp)(CO)HF$ **(76)**
Empirical formula	C35 H40 N2 O P2 Ru
Formula weight	667.70
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.3450(1)Å α = 99.123(1)^o
	b = 15.4690(2)Å β = 101.248(1)^o
	c = 20.8270(2)Å γ = 97.361(1)^o
Volume	3183.68(6) Å^3
Z	4
Density (calculated)	1.393 Mg/m^3
Absorption coefficient	0.623 mm^{-1}
F(000)	1384
Crystal size	0.33 x 0.13 x 0.10 mm
Theta range for data collection	3.75 to 27.47^o
Index ranges	-13<=h<=13; -20<=k<=20; -26<=l<=26
Reflections collected	62843
Independent reflections	14542 [R(int) = 0.0783]
Reflections observed (>2σ)	11194
Data Completeness	0.996
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.94 and 0.85
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14542 / 4 / 764
Goodness-of-fit on F^2	1.010
Final R indices [I>2σ(I)]	R1 = 0.0349 wR2 = 0.0801
R indices (all data)	R1 = 0.0554 wR2 = 0.0890
Largest diff. peak and hole	0.727 and -0.684 eÅ^{-3}

Table 107. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for $Ru(IMe_4)(dppp)(CO)HF$ **(76)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	8567(1)	6966(1)	866(1)	23(1)
P(1)	6893(1)	7574(1)	255(1)	24(1)
P(2)	8108(1)	7490(1)	1872(1)	23(1)
O(1)	11235(2)	8180(1)	1088(1)	47(1)
N(1)	9262(2)	6422(2)	-535(1)	32(1)
N(2)	8330(2)	5289(1)	-232(1)	31(1)
C(1)	10203(3)	7736(2)	987(1)	30(1)
C(2)	8782(2)	6176(2)	-12(1)	28(1)
C(3)	9071(3)	5718(2)	-1067(1)	39(1)
C(4)	8468(3)	5006(2)	-878(1)	38(1)
C(5)	9868(3)	7317(2)	-554(1)	40(1)

C(6)	9476(4)	5812(3)	-1706(2)	60(1)
C(7)	7910(3)	4087(2)	-1256(2)	54(1)
C(8)	7800(3)	4686(2)	155(2)	42(1)
C(9)	6382(2)	7696(2)	1867(1)	28(1)
C(10)	5777(3)	8204(2)	1335(1)	31(1)
C(11)	5415(2)	7651(2)	625(1)	30(1)
C(12)	6150(2)	6863(2)	-561(1)	27(1)
C(13)	6451(2)	7048(2)	-1153(1)	30(1)
C(14)	6002(3)	6429(2)	-1740(1)	35(1)
C(15)	5230(3)	5621(2)	-1755(1)	37(1)
C(16)	4924(3)	5433(2)	-1169(1)	37(1)
C(17)	5390(2)	6041(2)	-582(1)	34(1)
C(18)	7134(2)	8693(2)	53(1)	25(1)
C(19)	6128(3)	8990(2)	-365(1)	32(1)
C(20)	6298(3)	9849(2)	-489(1)	36(1)
C(21)	7487(3)	10421(2)	-199(1)	34(1)
C(22)	8489(3)	10136(2)	218(1)	33(1)
C(23)	8315(2)	9279(2)	344(1)	28(1)
C(24)	8220(2)	6767(2)	2499(1)	24(1)
C(25)	8191(2)	5861(2)	2316(1)	29(1)
C(26)	8233(3)	5319(2)	2793(1)	33(1)
C(27)	8305(2)	5681(2)	3452(1)	32(1)
C(28)	8349(3)	6585(2)	3641(1)	33(1)
C(29)	8296(2)	7122(2)	3166(1)	30(1)
C(30)	9164(2)	8507(2)	2382(1)	25(1)
C(31)	8720(3)	9269(2)	2627(1)	33(1)
C(32)	9613(3)	9997(2)	3025(1)	38(1)
C(33)	10950(3)	9954(2)	3183(1)	36(1)
C(34)	11421(3)	9198(2)	2946(1)	33(1)
C(35)	10534(2)	8480(2)	2544(1)	29(1)
Ru(1A)	6080(1)	2725(1)	4139(1)	22(1)
P(1A)	7097(1)	1818(1)	4806(1)	22(1)
P(2A)	5260(1)	1635(1)	3217(1)	23(1)
O(1A)	8300(2)	3591(1)	3571(1)	42(1)
N(1A)	7393(2)	4283(1)	5354(1)	26(1)
N(2A)	5316(2)	3933(1)	5319(1)	27(1)
C(1A)	7460(3)	3279(2)	3805(1)	29(1)
C(2A)	6271(2)	3726(2)	4982(1)	26(1)
C(3A)	7139(3)	4809(2)	5912(1)	30(1)
C(4A)	5827(3)	4578(2)	5891(1)	30(1)
C(5A)	8713(2)	4331(2)	5206(1)	37(1)
C(6A)	8181(3)	5465(2)	6402(2)	47(1)
C(7A)	5005(3)	4862(2)	6373(1)	42(1)
C(8A)	3897(2)	3553(2)	5112(1)	36(1)
C(9A)	5096(2)	482(2)	3358(1)	26(1)
C(10A)	6299(2)	267(2)	3831(1)	27(1)
C(11A)	6361(2)	629(2)	4570(1)	26(1)
C(12A)	6920(2)	2102(2)	5669(1)	25(1)
C(13A)	5687(3)	1875(2)	5834(1)	35(1)
C(14A)	5473(3)	2202(2)	6451(1)	43(1)
C(15A)	6469(3)	2774(2)	6926(1)	40(1)
C(16A)	7690(3)	3008(2)	6771(1)	36(1)
C(17A)	7915(2)	2674(2)	6151(1)	29(1)
C(18A)	8875(2)	1697(2)	4906(1)	24(1)
C(19A)	9609(2)	2000(2)	4473(1)	29(1)

C(20A)	10922(3)	1860(2)	4508(1)	35(1)
C(21A)	11505(3)	1405(2)	4977(1)	37(1)
C(22A)	10787(3)	1095(2)	5409(1)	35(1)
C(23A)	9476(2)	1238(2)	5379(1)	29(1)
C(24A)	6134(2)	1619(2)	2526(1)	24(1)
C(25A)	6535(2)	878(2)	2204(1)	34(1)
C(26A)	7125(3)	923(2)	1662(1)	38(1)
C(27A)	7301(3)	1710(2)	1432(1)	36(1)
C(28A)	6901(3)	2450(2)	1743(1)	35(1)
C(29A)	6327(2)	2410(2)	2289(1)	30(1)
C(30A)	3537(2)	1592(2)	2742(1)	26(1)
C(31A)	2688(2)	2130(2)	2975(1)	30(1)
C(32A)	1375(3)	2058(2)	2618(1)	37(1)
C(33A)	912(3)	1450(2)	2028(1)	39(1)
C(34A)	1746(3)	912(2)	1789(1)	40(1)
C(35A)	3056(3)	988(2)	2143(1)	35(1)

Table 108. Bond lengths [Å] and angles [°] for Ru(IMe_4)(dppp)(CO)HF **(76)**.

Ru(1)-C(1)	1.888(3)	Ru(1)-C(2)	2.099(2)
Ru(1)-P(2)	2.2849(6)	Ru(1)-P(1)	2.3320(6)
Ru(1)-H(1)	1.599(16)	Ru(1)-H(2)	1.626(17)
P(1)-C(12)	1.836(2)	P(1)-C(18)	1.844(2)
P(1)-C(11)	1.849(2)	P(2)-C(30)	1.837(2)
P(2)-C(24)	1.846(2)	P(2)-C(9)	1.851(2)
O(1)-C(1)	1.155(3)	N(1)-C(2)	1.367(3)
N(1)-C(3)	1.388(3)	N(1)-C(5)	1.454(3)
N(2)-C(2)	1.366(3)	N(2)-C(4)	1.388(3)
N(2)-C(8)	1.450(3)	C(3)-C(4)	1.347(4)
C(3)-C(6)	1.494(4)	C(4)-C(7)	1.494(4)
C(5)-H(5A)	0.9800	C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800	C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800	C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800	C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800	C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800	C(8)-H(8C)	0.9800
C(9)-C(10)	1.539(3)	C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900	C(10)-C(11)	1.535(3)
C(10)-H(10A)	0.9900	C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900	C(11)-H(11B)	0.9900
C(12)-C(13)	1.391(3)	C(12)-C(17)	1.397(4)
C(13)-C(14)	1.387(4)	C(13)-H(13)	0.9500
C(14)-C(15)	1.387(4)	C(14)-H(14)	0.9500
C(15)-C(16)	1.382(4)	C(15)-H(15)	0.9500
C(16)-C(17)	1.379(4)	C(16)-H(16)	0.9500
C(17)-H(17)	0.9500	C(18)-C(23)	1.391(3)
C(18)-C(19)	1.395(3)	C(19)-C(20)	1.388(4)
C(19)-H(19)	0.9500	C(20)-C(21)	1.387(4)
C(20)-H(20)	0.9500	C(21)-C(22)	1.383(4)
C(21)-H(21)	0.9500	C(22)-C(23)	1.386(3)
C(22)-H(22)	0.9500	C(23)-H(23)	0.9500
C(24)-C(25)	1.387(3)	C(24)-C(29)	1.395(3)
C(25)-C(26)	1.396(3)	C(25)-H(25)	0.9500
C(26)-C(27)	1.380(4)	C(26)-H(26)	0.9500
C(27)-C(28)	1.384(4)	C(27)-H(27)	0.9500

C(28)-C(29)	1.386(3)	C(28)-H(28)	0.9500
C(29)-H(29)	0.9500	C(30)-C(31)	1.378(4)
C(30)-C(35)	1.398(3)	C(31)-C(32)	1.396(4)
C(31)-H(31)	0.9500	C(32)-C(33)	1.371(4)
C(32)-H(32)	0.9500	C(33)-C(34)	1.379(4)
C(33)-H(33)	0.9500	C(34)-C(35)	1.387(4)
C(34)-H(34)	0.9500	C(35)-H(35)	0.9500
Ru(1A)-C(1A)	1.875(3)	Ru(1A)-C(2A)	2.107(2)
Ru(1A)-P(2A)	2.2859(6)	Ru(1A)-P(1A)	2.3301(6)
Ru(1A)-H(2A)	1.629(17)	Ru(1A)-H(1A)	1.615(16)
P(1A)-C(12A)	1.833(2)	P(1A)-C(18A)	1.847(2)
P(1A)-C(11A)	1.847(2)	P(2A)-C(24A)	1.841(2)
P(2A)-C(9A)	1.845(2)	P(2A)-C(30A)	1.850(2)
O(1A)-C(1A)	1.166(3)	N(1A)-C(2A)	1.367(3)
N(1A)-C(3A)	1.399(3)	N(1A)-C(5A)	1.454(3)
N(2A)-C(2A)	1.360(3)	N(2A)-C(4A)	1.393(3)
N(2A)-C(8A)	1.462(3)	C(3A)-C(4A)	1.348(4)
C(3A)-C(6A)	1.482(4)	C(4A)-C(7A)	1.487(4)
C(5A)-H(5A1)	0.9800	C(5A)-H(5A2)	0.9800
C(5A)-H(5A3)	0.9800	C(6A)-H(6A1)	0.9800
C(6A)-H(6A2)	0.9800	C(6A)-H(6A3)	0.9800
C(7A)-H(7A1)	0.9800	C(7A)-H(7A2)	0.9800
C(7A)-H(7A3)	0.9800	C(8A)-H(8A1)	0.9800
C(8A)-H(8A2)	0.9800	C(8A)-H(8A3)	0.9800
C(9A)-C(10A)	1.537(3)	C(9A)-H(9A1)	0.9900
C(9A)-H(9A2)	0.9900	C(10A)-C(11A)	1.536(3)
C(10A)-H(10C)	0.9900	C(10A)-H(10D)	0.9900
C(11A)-H(11C)	0.9900	C(11A)-H(11D)	0.9900
C(12A)-C(17A)	1.390(3)	C(12A)-C(13A)	1.401(3)
C(13A)-C(14A)	1.376(4)	C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.384(4)	C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.381(4)	C(15A)-H(15A)	0.9500
C(16A)-C(17A)	1.388(4)	C(16A)-H(16A)	0.9500
C(17A)-H(17A)	0.9500	C(18A)-C(19A)	1.386(3)
C(18A)-C(23A)	1.399(3)	C(19A)-C(20A)	1.393(3)
C(19A)-H(19A)	0.9500	C(20A)-C(21A)	1.383(4)
C(20A)-H(20A)	0.9500	C(21A)-C(22A)	1.378(4)
C(21A)-H(21A)	0.9500	C(22A)-C(23A)	1.393(3)
C(22A)-H(22A)	0.9500	C(23A)-H(23A)	0.9500
C(24A)-C(25A)	1.386(3)	C(24A)-C(29A)	1.395(3)
C(25A)-C(26A)	1.389(4)	C(25A)-H(25A)	0.9500
C(26A)-C(27A)	1.381(4)	C(26A)-H(26A)	0.9500
C(27A)-C(28A)	1.375(4)	C(27A)-H(27A)	0.9500
C(28A)-C(29A)	1.388(3)	C(28A)-H(28A)	0.9500
C(29A)-H(29A)	0.9500	C(30A)-C(31A)	1.387(3)
C(30A)-C(35A)	1.395(4)	C(31A)-C(32A)	1.396(3)
C(31A)-H(31A)	0.9500	C(32A)-C(33A)	1.383(4)
C(32A)-H(32A)	0.9500	C(33A)-C(34A)	1.381(4)
C(33A)-H(33A)	0.9500	C(34A)-C(35A)	1.392(4)
C(34A)-H(34A)	0.9500	C(35A)-H(35A)	0.9500
C(1)-Ru(1)-C(2)	94.70(10)	C(1)-Ru(1)-P(2)	96.77(8)
C(2)-Ru(1)-P(2)	165.51(7)	C(1)-Ru(1)-P(1)	108.07(8)
C(2)-Ru(1)-P(1)	90.51(6)	P(2)-Ru(1)-P(1)	94.30(2)
C(1)-Ru(1)-H(1)	87.5(10)	C(2)-Ru(1)-H(1)	87.1(10)

P(2)-Ru(1)-H(1)	84.6(9)	P(1)-Ru(1)-H(1)	164.4(10)
C(1)-Ru(1)-H(2)	173.7(9)	C(2)-Ru(1)-H(2)	86.9(9)
P(2)-Ru(1)-H(2)	80.8(9)	P(1)-Ru(1)-H(2)	77.9(9)
H(1)-Ru(1)-H(2)	86.5(13)	C(12)-P(1)-C(18)	102.97(11)
C(12)-P(1)-C(11)	101.83(11)	C(18)-P(1)-C(11)	98.97(11)
C(12)-P(1)-Ru(1)	111.56(8)	C(18)-P(1)-Ru(1)	124.21(8)
C(11)-P(1)-Ru(1)	114.39(8)	C(30)-P(2)-C(24)	99.36(10)
C(30)-P(2)-C(9)	104.06(11)	C(24)-P(2)-C(9)	97.59(11)
C(30)-P(2)-Ru(1)	117.79(8)	C(24)-P(2)-Ru(1)	117.84(8)
C(9)-P(2)-Ru(1)	116.89(8)	C(2)-N(1)-C(3)	112.2(2)
C(2)-N(1)-C(5)	125.0(2)	C(3)-N(1)-C(5)	122.8(2)
C(2)-N(2)-C(4)	112.2(2)	C(2)-N(2)-C(8)	125.4(2)
C(4)-N(2)-C(8)	122.4(2)	O(1)-C(1)-Ru(1)	176.1(2)
N(2)-C(2)-N(1)	102.7(2)	N(2)-C(2)-Ru(1)	127.47(18)
N(1)-C(2)-Ru(1)	129.50(18)	C(4)-C(3)-N(1)	106.4(2)
C(4)-C(3)-C(6)	130.5(3)	N(1)-C(3)-C(6)	123.0(3)
C(3)-C(4)-N(2)	106.5(2)	C(3)-C(4)-C(7)	131.1(3)
N(2)-C(4)-C(7)	122.2(3)	N(1)-C(5)-H(5A)	109.5
N(1)-C(5)-H(5B)	109.5	H(5A)-C(5)-H(5B)	109.5
N(1)-C(5)-H(5C)	109.5	H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5	C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5	H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5	H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5	C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5	H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5	H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5	N(2)-C(8)-H(8A)	109.5
N(2)-C(8)-H(8B)	109.5	H(8A)-C(8)-H(8B)	109.5
N(2)-C(8)-H(8C)	109.5	H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5	C(10)-C(9)-P(2)	116.12(17)
C(10)-C(9)-H(9A)	108.3	P(2)-C(9)-H(9A)	108.3
C(10)-C(9)-H(9B)	108.3	P(2)-C(9)-H(9B)	108.3
H(9A)-C(9)-H(9B)	107.4	C(11)-C(10)-C(9)	113.5(2)
C(11)-C(10)-H(10A)	108.9	C(9)-C(10)-H(10A)	108.9
C(11)-C(10)-H(10B)	108.9	C(9)-C(10)-H(10B)	108.9
H(10A)-C(10)-H(10B)	107.7	C(10)-C(11)-P(1)	112.41(17)
C(10)-C(11)-H(11A)	109.1	P(1)-C(11)-H(11A)	109.1
C(10)-C(11)-H(11B)	109.1	P(1)-C(11)-H(11B)	109.1
H(11A)-C(11)-H(11B)	107.9	C(13)-C(12)-C(17)	117.9(2)
C(13)-C(12)-P(1)	123.09(19)	C(17)-C(12)-P(1)	118.47(18)
C(14)-C(13)-C(12)	120.4(2)	C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8	C(13)-C(14)-C(15)	121.0(2)
C(13)-C(14)-H(14)	119.5	C(15)-C(14)-H(14)	119.5
C(16)-C(15)-C(14)	119.0(2)	C(16)-C(15)-H(15)	120.5
C(14)-C(15)-H(15)	120.5	C(17)-C(16)-C(15)	120.1(3)
C(17)-C(16)-H(16)	120.0	C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(12)	121.6(2)	C(16)-C(17)-H(17)	119.2
C(12)-C(17)-H(17)	119.2	C(23)-C(18)-C(19)	118.4(2)
C(23)-C(18)-P(1)	120.03(17)	C(19)-C(18)-P(1)	121.53(19)
C(20)-C(19)-C(18)	121.0(2)	C(20)-C(19)-H(19)	119.5
C(18)-C(19)-H(19)	119.5	C(21)-C(20)-C(19)	119.8(2)
C(21)-C(20)-H(20)	120.1	C(19)-C(20)-H(20)	120.1
C(22)-C(21)-C(20)	119.7(2)	C(22)-C(21)-H(21)	120.2
C(20)-C(21)-H(21)	120.2	C(21)-C(22)-C(23)	120.4(2)
C(21)-C(22)-H(22)	119.8	C(23)-C(22)-H(22)	119.8

C(22)-C(23)-C(18)	120.7(2)	C(22)-C(23)-H(23)	119.6
C(18)-C(23)-H(23)	119.6	C(25)-C(24)-C(29)	118.7(2)
C(25)-C(24)-P(2)	121.12(18)	C(29)-C(24)-P(2)	120.17(18)
C(24)-C(25)-C(26)	120.3(2)	C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8	C(27)-C(26)-C(25)	120.3(2)
C(27)-C(26)-H(26)	119.9	C(25)-C(26)-H(26)	119.9
C(26)-C(27)-C(28)	119.9(2)	C(26)-C(27)-H(27)	120.1
C(28)-C(27)-H(27)	120.1	C(27)-C(28)-C(29)	119.9(2)
C(27)-C(28)-H(28)	120.1	C(29)-C(28)-H(28)	120.1
C(28)-C(29)-C(24)	120.9(2)	C(28)-C(29)-H(29)	119.5
C(24)-C(29)-H(29)	119.5	C(31)-C(30)-C(35)	118.4(2)
C(31)-C(30)-P(2)	125.80(19)	C(35)-C(30)-P(2)	115.79(18)
C(30)-C(31)-C(32)	120.9(2)	C(30)-C(31)-H(31)	119.5
C(32)-C(31)-H(31)	119.5	C(33)-C(32)-C(31)	119.8(3)
C(33)-C(32)-H(32)	120.1	C(31)-C(32)-H(32)	120.1
C(32)-C(33)-C(34)	120.5(3)	C(32)-C(33)-H(33)	119.8
C(34)-C(33)-H(33)	119.8	C(33)-C(34)-C(35)	119.7(2)
C(33)-C(34)-H(34)	120.2	C(35)-C(34)-H(34)	120.2
C(34)-C(35)-C(30)	120.8(2)	C(34)-C(35)-H(35)	119.6
C(30)-C(35)-H(35)	119.6	C(1A)-Ru(1A)-C(2A)	96.49(10)
C(1A)-Ru(1A)-P(2A)	95.66(8)	C(2A)-Ru(1A)-P(2A)	164.16(7)
C(1A)-Ru(1A)-P(1A)	104.73(7)	C(2A)-Ru(1A)-P(1A)	90.76(6)
P(2A)-Ru(1A)-P(1A)	95.93(2)	C(1A)-Ru(1A)-H(2A)	174.5(9)
C(2A)-Ru(1A)-H(2A)	86.9(10)	P(2A)-Ru(1A)-H(2A)	80.2(10)
P(1A)-Ru(1A)-H(2A)	79.5(9)	C(1A)-Ru(1A)-H(1A)	91.7(9)
C(2A)-Ru(1A)-H(1A)	85.2(9)	P(2A)-Ru(1A)-H(1A)	84.4(9)
P(1A)-Ru(1A)-H(1A)	163.4(9)	H(2A)-Ru(1A)-H(1A)	84.2(13)
C(12A)-P(1A)-C(18A)	102.80(10)	C(12A)-P(1A)-C(11A)	102.73(11)
C(18A)-P(1A)-C(11A)	98.26(11)	C(12A)-P(1A)-Ru(1A)	111.67(7)
C(18A)-P(1A)-Ru(1A)	123.73(8)	C(11A)-P(1A)-Ru(1A)	114.88(8)
C(24A)-P(2A)-C(9A)	104.15(11)	C(24A)-P(2A)-C(30A)	98.97(10)
C(9A)-P(2A)-C(30A)	98.18(11)	C(24A)-P(2A)-Ru(1A)	117.47(8)
C(9A)-P(2A)-Ru(1A)	116.42(8)	C(30A)-P(2A)-Ru(1A)	118.46(8)
C(2A)-N(1A)-C(3A)	112.2(2)	C(2A)-N(1A)-C(5A)	125.2(2)
C(3A)-N(1A)-C(5A)	122.6(2)	C(2A)-N(2A)-C(4A)	112.5(2)
C(2A)-N(2A)-C(8A)	125.4(2)	C(4A)-N(2A)-C(8A)	122.2(2)
O(1A)-C(1A)-Ru(1A)	176.7(2)	N(2A)-C(2A)-N(1A)	102.8(2)
N(2A)-C(2A)-Ru(1A)	128.09(18)	N(1A)-C(2A)-Ru(1A)	128.99(17)
C(4A)-C(3A)-N(1A)	106.1(2)	C(4A)-C(3A)-C(6A)	130.6(3)
N(1A)-C(3A)-C(6A)	123.4(2)	C(3A)-C(4A)-N(2A)	106.5(2)
C(3A)-C(4A)-C(7A)	130.8(3)	N(2A)-C(4A)-C(7A)	122.6(2)
N(1A)-C(5A)-H(5A1)	109.5	N(1A)-C(5A)-H(5A2)	109.5
H(5A1)-C(5A)-H(5A2)	109.5	N(1A)-C(5A)-H(5A3)	109.5
H(5A1)-C(5A)-H(5A3)	109.5	H(5A2)-C(5A)-H(5A3)	109.5
C(3A)-C(6A)-H(6A1)	109.5	C(3A)-C(6A)-H(6A2)	109.5
H(6A1)-C(6A)-H(6A2)	109.5	C(3A)-C(6A)-H(6A3)	109.5
H(6A1)-C(6A)-H(6A3)	109.5	H(6A2)-C(6A)-H(6A3)	109.5
C(4A)-C(7A)-H(7A1)	109.5	C(4A)-C(7A)-H(7A2)	109.5
H(7A1)-C(7A)-H(7A2)	109.5	C(4A)-C(7A)-H(7A3)	109.5
H(7A1)-C(7A)-H(7A3)	109.5	H(7A2)-C(7A)-H(7A3)	109.5
N(2A)-C(8A)-H(8A1)	109.5	N(2A)-C(8A)-H(8A2)	109.5
H(8A1)-C(8A)-H(8A2)	109.5	N(2A)-C(8A)-H(8A3)	109.5
H(8A1)-C(8A)-H(8A3)	109.5	H(8A2)-C(8A)-H(8A3)	109.5
C(10A)-C(9A)-P(2A)	115.13(16)	C(10A)-C(9A)-H(9A1)	108.5
P(2A)-C(9A)-H(9A1)	108.5	C(10A)-C(9A)-H(9A2)	108.5

P(2A)-C(9A)-H(9A2)	108.5	H(9A1)-C(9A)-H(9A2)	107.5
C(11A)-C(10A)-C(9A)	113.3(2)	C(11A)-C(10A)-H(10C)	108.9
C(9A)-C(10A)-H(10C)	108.9	C(11A)-C(10A)-H(10D)	108.9
C(9A)-C(10A)-H(10D)	108.9	H(10C)-C(10A)-H(10D)	107.7
C(10A)-C(11A)-P(1A)	111.45(16)	C(10A)-C(11A)-H(11C)	109.3
P(1A)-C(11A)-H(11C)	109.3	C(10A)-C(11A)-H(11D)	109.3
P(1A)-C(11A)-H(11D)	109.3	H(11C)-C(11A)-H(11D)	108.0
C(17A)-C(12A)-C(13A)	117.5(2)	C(17A)-C(12A)-P(1A)	121.27(18)
C(13A)-C(12A)-P(1A)	120.30(19)	C(14A)-C(13A)-C(12A)	121.2(3)
C(14A)-C(13A)-H(13A)	119.4	C(12A)-C(13A)-H(13A)	119.4
C(13A)-C(14A)-C(15A)	120.8(3)	C(13A)-C(14A)-H(14A)	119.6
C(15A)-C(14A)-H(14A)	119.6	C(16A)-C(15A)-C(14A)	118.8(3)
C(16A)-C(15A)-H(15A)	120.6	C(14A)-C(15A)-H(15A)	120.6
C(15A)-C(16A)-C(17A)	120.6(3)	C(15A)-C(16A)-H(16A)	119.7
C(17A)-C(16A)-H(16A)	119.7	C(16A)-C(17A)-C(12A)	121.1(2)
C(16A)-C(17A)-H(17A)	119.5	C(12A)-C(17A)-H(17A)	119.5
C(19A)-C(18A)-C(23A)	118.6(2)	C(19A)-C(18A)-P(1A)	119.97(17)
C(23A)-C(18A)-P(1A)	121.23(18)	C(18A)-C(19A)-C(20A)	121.1(2)
C(18A)-C(19A)-H(19A)	119.5	C(20A)-C(19A)-H(19A)	119.5
C(21A)-C(20A)-C(19A)	119.7(2)	C(21A)-C(20A)-H(20A)	120.1
C(19A)-C(20A)-H(20A)	120.1	C(22A)-C(21A)-C(20A)	119.9(2)
C(22A)-C(21A)-H(21A)	120.0	C(20A)-C(21A)-H(21A)	120.0
C(21A)-C(22A)-C(23A)	120.5(2)	C(21A)-C(22A)-H(22A)	119.7
C(23A)-C(22A)-H(22A)	119.7	C(22A)-C(23A)-C(18A)	120.1(2)
C(22A)-C(23A)-H(23A)	119.9	C(18A)-C(23A)-H(23A)	119.9
C(25A)-C(24A)-C(29A)	118.3(2)	C(25A)-C(24A)-P(2A)	125.29(19)
C(29A)-C(24A)-P(2A)	116.27(18)	C(24A)-C(25A)-C(26A)	120.9(2)
C(24A)-C(25A)-H(25A)	119.5	C(26A)-C(25A)-H(25A)	119.5
C(27A)-C(26A)-C(25A)	120.0(3)	C(27A)-C(26A)-H(26A)	120.0
C(25A)-C(26A)-H(26A)	120.0	C(28A)-C(27A)-C(26A)	119.8(2)
C(28A)-C(27A)-H(27A)	120.1	C(26A)-C(27A)-H(27A)	120.1
C(27A)-C(28A)-C(29A)	120.3(2)	C(27A)-C(28A)-H(28A)	119.9
C(29A)-C(28A)-H(28A)	119.9	C(28A)-C(29A)-C(24A)	120.6(2)
C(28A)-C(29A)-H(29A)	119.7	C(24A)-C(29A)-H(29A)	119.7
C(31A)-C(30A)-C(35A)	118.6(2)	C(31A)-C(30A)-P(2A)	121.72(19)
C(35A)-C(30A)-P(2A)	119.61(18)	C(30A)-C(31A)-C(32A)	120.4(2)
C(30A)-C(31A)-H(31A)	119.8	C(32A)-C(31A)-H(31A)	119.8
C(33A)-C(32A)-C(31A)	120.1(2)	C(33A)-C(32A)-H(32A)	119.9
C(31A)-C(32A)-H(32A)	119.9	C(34A)-C(33A)-C(32A)	120.1(2)
C(34A)-C(33A)-H(33A)	119.9	C(32A)-C(33A)-H(33A)	119.9
C(33A)-C(34A)-C(35A)	119.6(3)	C(33A)-C(34A)-H(34A)	120.2
C(35A)-C(34A)-H(34A)	120.2	C(34A)-C(35A)-C(30A)	121.0(2)
C(34A)-C(35A)-H(35A)	119.5	C(30A)-C(35A)-H(35A)	119.5

Table 109. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(IMe_4)(dppp)(CO)HF$ **(76)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	22(1)	25(1)	21(1)	5(1)	4(1)	2(1)
P(1)	23(1)	27(1)	22(1)	6(1)	3(1)	1(1)
P(2)	24(1)	24(1)	21(1)	5(1)	3(1)	2(1)
O(1)	32(1)	59(1)	45(1)	17(1)	5(1)	-13(1)
N(1)	33(1)	39(1)	26(1)	6(1)	10(1)	11(1)

N(2)	25(1)	30(1)	34(1)	-1(1)	4(1)	5(1)
C(1)	33(2)	33(1)	25(1)	8(1)	7(1)	4(1)
C(2)	23(1)	32(1)	29(1)	4(1)	3(1)	6(1)
C(3)	35(2)	55(2)	26(1)	-1(1)	5(1)	16(1)
C(4)	25(1)	49(2)	34(2)	-7(1)	0(1)	14(1)
C(5)	47(2)	46(2)	35(2)	17(1)	19(1)	9(1)
C(6)	66(2)	80(3)	35(2)	3(2)	18(2)	22(2)
C(7)	35(2)	55(2)	57(2)	-21(2)	4(1)	6(2)
C(8)	41(2)	32(2)	50(2)	6(1)	9(1)	0(1)
C(9)	24(1)	35(1)	26(1)	6(1)	7(1)	4(1)
C(10)	28(1)	39(2)	30(1)	7(1)	8(1)	12(1)
C(11)	24(1)	38(2)	27(1)	8(1)	5(1)	4(1)
C(12)	24(1)	32(1)	23(1)	6(1)	1(1)	4(1)
C(13)	27(1)	32(1)	29(1)	7(1)	4(1)	2(1)
C(14)	35(2)	46(2)	25(1)	9(1)	7(1)	10(1)
C(15)	36(2)	40(2)	28(1)	-4(1)	1(1)	4(1)
C(16)	33(2)	35(2)	38(2)	2(1)	2(1)	-5(1)
C(17)	30(1)	40(2)	28(1)	7(1)	3(1)	0(1)
C(18)	27(1)	28(1)	21(1)	4(1)	6(1)	5(1)
C(19)	32(1)	33(2)	29(1)	6(1)	1(1)	3(1)
C(20)	47(2)	38(2)	26(1)	11(1)	6(1)	14(1)
C(21)	48(2)	27(1)	34(1)	10(1)	18(1)	9(1)
C(22)	32(1)	31(1)	36(1)	2(1)	14(1)	2(1)
C(23)	26(1)	31(1)	26(1)	5(1)	5(1)	5(1)
C(24)	20(1)	27(1)	23(1)	6(1)	2(1)	-1(1)
C(25)	32(1)	30(1)	23(1)	4(1)	2(1)	1(1)
C(26)	35(1)	27(1)	34(1)	8(1)	6(1)	2(1)
C(27)	28(1)	40(2)	30(1)	17(1)	4(1)	1(1)
C(28)	33(1)	39(2)	23(1)	6(1)	5(1)	-1(1)
C(29)	32(1)	28(1)	28(1)	4(1)	6(1)	-1(1)
C(30)	26(1)	28(1)	19(1)	7(1)	4(1)	0(1)
C(31)	32(1)	31(1)	35(1)	6(1)	4(1)	5(1)
C(32)	46(2)	24(1)	42(2)	1(1)	9(1)	4(1)
C(33)	43(2)	28(1)	32(1)	2(1)	5(1)	-7(1)
C(34)	28(1)	34(2)	34(1)	7(1)	2(1)	-1(1)
C(35)	30(1)	26(1)	28(1)	5(1)	5(1)	3(1)
Ru(1A)	22(1)	22(1)	21(1)	6(1)	2(1)	2(1)
P(1A)	21(1)	24(1)	20(1)	6(1)	3(1)	1(1)
P(2A)	20(1)	26(1)	21(1)	5(1)	2(1)	3(1)
O(1A)	44(1)	41(1)	40(1)	16(1)	11(1)	-7(1)
N(1A)	26(1)	25(1)	26(1)	5(1)	3(1)	-2(1)
N(2A)	25(1)	24(1)	31(1)	5(1)	6(1)	3(1)
C(1A)	37(1)	25(1)	23(1)	8(1)	1(1)	4(1)
C(2A)	27(1)	24(1)	26(1)	7(1)	2(1)	4(1)
C(3A)	38(2)	24(1)	27(1)	4(1)	5(1)	1(1)
C(4A)	39(2)	24(1)	29(1)	4(1)	9(1)	5(1)
C(5A)	24(1)	47(2)	35(2)	4(1)	2(1)	-5(1)
C(6A)	47(2)	43(2)	40(2)	-6(1)	2(1)	-4(1)
C(7A)	50(2)	33(2)	44(2)	1(1)	19(1)	4(1)
C(8A)	25(1)	40(2)	42(2)	2(1)	10(1)	3(1)
C(9A)	25(1)	26(1)	22(1)	4(1)	2(1)	-1(1)
C(10A)	27(1)	22(1)	28(1)	5(1)	4(1)	1(1)
C(11A)	28(1)	25(1)	25(1)	9(1)	3(1)	1(1)
C(12A)	27(1)	26(1)	24(1)	9(1)	6(1)	6(1)
C(13A)	35(2)	37(2)	31(1)	3(1)	9(1)	-2(1)

C(14A)	43(2)	48(2)	42(2)	8(1)	24(1)	1(1)
C(15A)	54(2)	39(2)	28(1)	4(1)	16(1)	7(1)
C(16A)	45(2)	33(2)	28(1)	2(1)	4(1)	5(1)
C(17A)	28(1)	32(1)	27(1)	7(1)	6(1)	6(1)
C(18A)	22(1)	22(1)	23(1)	1(1)	1(1)	1(1)
C(19A)	28(1)	29(1)	28(1)	5(1)	6(1)	2(1)
C(20A)	30(1)	33(2)	38(2)	-3(1)	11(1)	-2(1)
C(21A)	23(1)	35(2)	45(2)	-7(1)	2(1)	8(1)
C(22A)	34(1)	29(1)	33(1)	-2(1)	-7(1)	7(1)
C(23A)	29(1)	28(1)	27(1)	3(1)	1(1)	3(1)
C(24A)	17(1)	31(1)	19(1)	2(1)	1(1)	1(1)
C(25A)	29(1)	34(2)	39(2)	8(1)	8(1)	7(1)
C(26A)	31(1)	44(2)	43(2)	2(1)	14(1)	11(1)
C(27A)	27(1)	50(2)	30(1)	6(1)	9(1)	2(1)
C(28A)	34(1)	41(2)	30(1)	13(1)	6(1)	5(1)
C(29A)	29(1)	36(2)	25(1)	8(1)	2(1)	6(1)
C(30A)	22(1)	36(1)	22(1)	12(1)	3(1)	3(1)
C(31A)	26(1)	34(1)	31(1)	11(1)	4(1)	4(1)
C(32A)	26(1)	44(2)	47(2)	18(1)	10(1)	10(1)
C(33A)	21(1)	57(2)	35(2)	20(1)	-3(1)	1(1)
C(34A)	30(1)	57(2)	27(1)	6(1)	-2(1)	-1(1)
C(35A)	30(1)	46(2)	26(1)	6(1)	4(1)	6(1)

Table 110. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(IMe$_4$)(dppp)(CO)HF **(76)**.

Atom	x	y	z	U(eq)
H(5A)	9505	7747	-270	60
H(5B)	9669	7417	-1013	60
H(5C)	10838	7388	-392	60
H(6A)	9295	5230	-2001	89
H(6B)	10432	6049	-1614	89
H(6C)	8965	6219	-1922	89
H(7A)	8107	4023	-1702	81
H(7B)	6941	3977	-1298	81
H(7C)	8318	3657	-1018	81
H(8A)	8057	4960	629	63
H(8B)	8162	4132	85	63
H(8C)	6824	4559	14	63
H(9A)	5797	7116	1803	34
H(9B)	6370	8033	2311	34
H(10A)	4962	8403	1446	38
H(10B)	6424	8739	1347	38
H(11A)	4763	7922	340	36
H(11B)	4984	7046	636	36
H(13)	6966	7602	-1154	36
H(14)	6228	6560	-2139	42
H(15)	4915	5204	-2160	44
H(16)	4392	4883	-1171	45
H(17)	5189	5897	-182	40
H(19)	5314	8599	-568	39
H(20)	5602	10043	-771	43
H(21)	7612	11007	-286	41
H(22)	9301	10528	420	39

H(23)	9010	9091	632	33
H(25)	8141	5608	1864	35
H(26)	8212	4700	2664	39
H(27)	8325	5309	3774	39
H(28)	8415	6837	4095	39
H(29)	8312	7741	3297	36
H(31)	7792	9298	2524	40
H(32)	9295	10521	3185	46
H(33)	11556	10447	3457	44
H(34)	12348	9171	3057	40
H(35)	10860	7962	2376	34
H(1)	9390(20)	6334(16)	1264(12)	39(7)
H(2)	7240(20)	6256(15)	827(13)	42(8)
H(2A)	4790(20)	2234(17)	4358(13)	44(8)
H(1A)	5020(20)	3265(16)	3771(12)	38(7)
H(5A1)	8880	3730	5056	55
H(5A2)	9388	4618	5608	55
H(5A3)	8763	4677	4853	55
H(6A1)	7772	5783	6735	70
H(6A2)	8605	5889	6172	70
H(6A3)	8857	5156	6625	70
H(7A1)	5569	5287	6754	63
H(7A2)	4616	4343	6527	63
H(7A3)	4288	5142	6153	63
H(8A1)	3684	3282	4637	54
H(8A2)	3361	4022	5186	54
H(8A3)	3696	3099	5373	54
H(9A1)	4292	357	3540	31
H(9A2)	4950	77	2922	31
H(10C)	6254	-385	3765	32
H(10D)	7131	521	3715	32
H(11C)	6905	288	4850	31
H(11D)	5448	548	4654	31
H(13A)	4986	1489	5513	42
H(14A)	4632	2032	6553	51
H(15A)	6317	3002	7351	48
H(16A)	8381	3402	7092	44
H(17A)	8763	2838	6055	35
H(19A)	9209	2307	4146	34
H(20A)	11416	2077	4210	42
H(21A)	12400	1307	5002	44
H(22A)	11189	781	5730	42
H(23A)	8990	1024	5680	35
H(25A)	6406	333	2356	40
H(26A)	7406	412	1451	46
H(27A)	7697	1740	1059	43
H(28A)	7019	2990	1583	42
H(29A)	6062	2926	2504	36
H(31A)	3002	2550	3379	36
H(32A)	799	2427	2782	44
H(33A)	18	1403	1787	46
H(34A)	1427	492	1385	48
H(35A)	3633	624	1974	41

Table 111. Dihedral angles [°] for Ru(IMe$_4$)(dppp)(CO)HF **(76)**.

Atom1 - Atom2 - Atom3 - Atom4	Dihedral
C(1) - Ru(1) - P(1) - C(12)	115.59(12)
C(2) - Ru(1) - P(1) - C(12)	20.47(11)
P(2) - Ru(1) - P(1) - C(12)	-145.85(9)
C(1) - Ru(1) - P(1) - C(18)	-8.49(12)
C(2) - Ru(1) - P(1) - C(18)	-103.61(12)
P(2) - Ru(1) - P(1) - C(18)	90.07(9)
C(1) - Ru(1) - P(1) - C(11)	-129.51(12)
C(2) - Ru(1) - P(1) - C(11)	135.38(12)
P(2) - Ru(1) - P(1) - C(11)	-30.95(10)
C(1) - Ru(1) - P(2) - C(30)	9.50(11)
C(2) - Ru(1) - P(2) - C(30)	151.6(3)
P(1) - Ru(1) - P(2) - C(30)	-99.29(9)
C(1) - Ru(1) - P(2) - C(24)	-109.58(11)
C(2) - Ru(1) - P(2) - C(24)	32.5(3)
P(1) - Ru(1) - P(2) - C(24)	141.62(9)
C(1) - Ru(1) - P(2) - C(9)	134.61(12)
C(2) - Ru(1) - P(2) - C(9)	-83.3(3)
P(1) - Ru(1) - P(2) - C(9)	25.81(10)
C(2) - Ru(1) - C(1) - O(1)	-100(4)
P(2) - Ru(1) - C(1) - O(1)	71(4)
P(1) - Ru(1) - C(1) - O(1)	168(4)
C(4) - N(2) - C(2) - N(1)	-2.7(3)
C(8) - N(2) - C(2) - N(1)	175.4(2)
C(4) - N(2) - C(2) - Ru(1)	170.93(17)
C(8) - N(2) - C(2) - Ru(1)	-10.9(3)
C(3) - N(1) - C(2) - N(2)	2.0(3)
C(5) - N(1) - C(2) - N(2)	-179.8(2)
C(3) - N(1) - C(2) - Ru(1)	-171.49(17)
C(5) - N(1) - C(2) - Ru(1)	6.7(4)
C(1) - Ru(1) - C(2) - N(2)	147.9(2)
P(2) - Ru(1) - C(2) - N(2)	5.6(4)
P(1) - Ru(1) - C(2) - N(2)	-103.9(2)
C(1) - Ru(1) - C(2) - N(1)	-40.1(2)
P(2) - Ru(1) - C(2) - N(1)	177.62(14)
P(1) - Ru(1) - C(2) - N(1)	68.1(2)
C(2) - N(1) - C(3) - C(4)	-0.6(3)
C(5) - N(1) - C(3) - C(4)	-178.8(2)
C(2) - N(1) - C(3) - C(6)	178.6(2)
C(5) - N(1) - C(3) - C(6)	0.3(4)
N(1) - C(3) - C(4) - N(2)	-1.1(3)
C(6) - C(3) - C(4) - N(2)	179.8(3)
N(1) - C(3) - C(4) - C(7)	174.0(3)
C(6) - C(3) - C(4) - C(7)	-5.0(5)
C(2) - N(2) - C(4) - C(3)	2.5(3)
C(8) - N(2) - C(4) - C(3)	-175.7(2)
C(2) - N(2) - C(4) - C(7)	-173.2(2)
C(8) - N(2) - C(4) - C(7)	8.6(4)
C(30) - P(2) - C(9) - C(10)	85.3(2)
C(24) - P(2) - C(9) - C(10)	-173.03(19)
Ru(1) - P(2) - C(9) - C(10)	-46.5(2)
P(2) - C(9) - C(10) - C(11)	72.4(3)

C(9) - C(10) - C(11) - P(1)	-78.5(2)
C(12) - P(1) - C(11) - C(10)	178.47(17)
C(18) - P(1) - C(11) - C(10)	-76.15(19)
Ru(1) - P(1) - C(11) - C(10)	58.00(19)
C(18) - P(1) - C(12) - C(13)	32.2(2)
C(11) - P(1) - C(12) - C(13)	134.4(2)
Ru(1) - P(1) - C(12) - C(13)	-103.1(2)
C(18) - P(1) - C(12) - C(17)	-156.61(19)
C(11) - P(1) - C(12) - C(17)	-54.4(2)
Ru(1) - P(1) - C(12) - C(17)	68.1(2)
C(17) - C(12) - C(13) - C(14)	0.0(3)
P(1) - C(12) - C(13) - C(14)	171.23(19)
C(12) - C(13) - C(14) - C(15)	1.1(4)
C(13) - C(14) - C(15) - C(16)	-0.9(4)
C(14) - C(15) - C(16) - C(17)	-0.3(4)
C(15) - C(16) - C(17) - C(12)	1.4(4)
C(13) - C(12) - C(17) - C(16)	-1.2(4)
P(1) - C(12) - C(17) - C(16)	-172.9(2)
C(12) - P(1) - C(18) - C(23)	-136.8(2)
C(11) - P(1) - C(18) - C(23)	118.8(2)
Ru(1) - P(1) - C(18) - C(23)	-9.0(2)
C(12) - P(1) - C(18) - C(19)	46.3(2)
C(11) - P(1) - C(18) - C(19)	-58.1(2)
Ru(1) - P(1) - C(18) - C(19)	174.11(16)
C(23) - C(18) - C(19) - C(20)	0.0(4)
P(1) - C(18) - C(19) - C(20)	176.9(2)
C(18) - C(19) - C(20) - C(21)	0.5(4)
C(19) - C(20) - C(21) - C(22)	-0.7(4)
C(20) - C(21) - C(22) - C(23)	0.5(4)
C(21) - C(22) - C(23) - C(18)	0.1(4)
C(19) - C(18) - C(23) - C(22)	-0.3(4)
P(1) - C(18) - C(23) - C(22)	-177.28(18)
C(30) - P(2) - C(24) - C(25)	-147.1(2)
C(9) - P(2) - C(24) - C(25)	107.2(2)
Ru(1) - P(2) - C(24) - C(25)	-18.7(2)
C(30) - P(2) - C(24) - C(29)	34.9(2)
C(9) - P(2) - C(24) - C(29)	-70.8(2)
Ru(1) - P(2) - C(24) - C(29)	163.33(16)
C(29) - C(24) - C(25) - C(26)	0.2(4)
P(2) - C(24) - C(25) - C(26)	-177.89(19)
C(24) - C(25) - C(26) - C(27)	0.0(4)
C(25) - C(26) - C(27) - C(28)	-0.6(4)
C(26) - C(27) - C(28) - C(29)	1.1(4)
C(27) - C(28) - C(29) - C(24)	-1.0(4)
C(25) - C(24) - C(29) - C(28)	0.4(4)
P(2) - C(24) - C(29) - C(28)	178.42(19)
C(24) - P(2) - C(30) - C(31)	-107.0(2)
C(9) - P(2) - C(30) - C(31)	-6.6(2)
Ru(1) - P(2) - C(30) - C(31)	124.6(2)
C(24) - P(2) - C(30) - C(35)	71.20(19)
C(9) - P(2) - C(30) - C(35)	171.53(18)
Ru(1) - P(2) - C(30) - C(35)	-57.25(19)
C(35) - C(30) - C(31) - C(32)	0.3(4)
P(2) - C(30) - C(31) - C(32)	178.4(2)
C(30) - C(31) - C(32) - C(33)	-0.9(4)

C(31) - C(32) - C(33) - C(34)	0.7(4)
C(32) - C(33) - C(34) - C(35)	0.1(4)
C(33) - C(34) - C(35) - C(30)	-0.8(4)
C(31) - C(30) - C(35) - C(34)	0.5(4)
P(2) - C(30) - C(35) - C(34)	-177.78(19)
C(1A) - Ru(1A) - P(1A) - C(12A)	121.06(12)
C(2A) - Ru(1A) - P(1A) - C(12A)	24.14(11)
P(2A) - Ru(1A) - P(1A) - C(12A)	-141.49(9)
C(1A) - Ru(1A) - P(1A) - C(18A)	-2.45(12)
C(2A) - Ru(1A) - P(1A) - C(18A)	-99.37(11)
P(2A) - Ru(1A) - P(1A) - C(18A)	95.00(9)
C(1A) - Ru(1A) - P(1A) - C(11A)	-122.47(12)
C(2A) - Ru(1A) - P(1A) - C(11A)	140.61(11)
P(2A) - Ru(1A) - P(1A) - C(11A)	-25.01(9)
C(1A) - Ru(1A) - P(2A) - C(24A)	1.67(11)
C(2A) - Ru(1A) - P(2A) - C(24A)	141.6(2)
P(1A) - Ru(1A) - P(2A) - C(24A)	-103.82(8)
C(1A) - Ru(1A) - P(2A) - C(9A)	126.14(11)
C(2A) - Ru(1A) - P(2A) - C(9A)	-93.9(2)
P(1A) - Ru(1A) - P(2A) - C(9A)	20.64(9)
C(1A) - Ru(1A) - P(2A) - C(30A)	-117.12(11)
C(2A) - Ru(1A) - P(2A) - C(30A)	22.9(3)
P(1A) - Ru(1A) - P(2A) - C(30A)	137.38(9)
C(2A) - Ru(1A) - C(1A) - O(1A)	-173(4)
P(2A) - Ru(1A) - C(1A) - O(1A)	-3(4)
P(1A) - Ru(1A) - C(1A) - O(1A)	95(4)
C(4A) - N(2A) - C(2A) - N(1A)	-1.7(3)
C(8A) - N(2A) - C(2A) - N(1A)	176.9(2)
C(4A) - N(2A) - C(2A) - Ru(1A)	174.25(16)
C(8A) - N(2A) - C(2A) - Ru(1A)	-7.2(3)
C(3A) - N(1A) - C(2A) - N(2A)	1.0(3)
C(5A) - N(1A) - C(2A) - N(2A)	-179.8(2)
C(3A) - N(1A) - C(2A) - Ru(1A)	-174.85(16)
C(5A) - N(1A) - C(2A) - Ru(1A)	4.3(3)
C(1A) - Ru(1A) - C(2A) - N(2A)	153.5(2)
P(2A) - Ru(1A) - C(2A) - N(2A)	13.6(4)
P(1A) - Ru(1A) - C(2A) - N(2A)	-101.6(2)
C(1A) - Ru(1A) - C(2A) - N(1A)	-31.7(2)
P(2A) - Ru(1A) - C(2A) - N(1A)	-171.56(13)
P(1A) - Ru(1A) - C(2A) - N(1A)	73.3(2)
C(2A) - N(1A) - C(3A) - C(4A)	0.0(3)
C(5A) - N(1A) - C(3A) - C(4A)	-179.2(2)
C(2A) - N(1A) - C(3A) - C(6A)	179.4(2)
C(5A) - N(1A) - C(3A) - C(6A)	0.2(4)
N(1A) - C(3A) - C(4A) - N(2A)	-1.0(3)
C(6A) - C(3A) - C(4A) - N(2A)	179.7(3)
N(1A) - C(3A) - C(4A) - C(7A)	175.1(3)
C(6A) - C(3A) - C(4A) - C(7A)	-4.2(5)
C(2A) - N(2A) - C(4A) - C(3A)	1.7(3)
C(8A) - N(2A) - C(4A) - C(3A)	-176.9(2)
C(2A) - N(2A) - C(4A) - C(7A)	-174.8(2)
C(8A) - N(2A) - C(4A) - C(7A)	6.6(4)
C(24A) - P(2A) - C(9A) - C(10A)	86.48(18)
C(30A) - P(2A) - C(9A) - C(10A)	-172.06(18)
Ru(1A) - P(2A) - C(9A) - C(10A)	-44.5(2)

P(2A) - C(9A) - C(10A) - C(11A)	76.5(2)
C(9A) - C(10A) - C(11A) - P(1A)	-81.1(2)
C(12A) - P(1A) - C(11A) - C(10A)	175.16(16)
C(18A) - P(1A) - C(11A) - C(10A)	-79.63(17)
Ru(1A) - P(1A) - C(11A) - C(10A)	53.68(18)
C(18A) - P(1A) - C(12A) - C(17A)	39.7(2)
C(11A) - P(1A) - C(12A) - C(17A)	141.34(19)
Ru(1A) - P(1A) - C(12A) - C(17A)	-95.02(19)
C(18A) - P(1A) - C(12A) - C(13A)	-151.6(2)
C(11A) - P(1A) - C(12A) - C(13A)	-49.9(2)
Ru(1A) - P(1A) - C(12A) - C(13A)	73.7(2)
C(17A) - C(12A) - C(13A) - C(14A)	-0.4(4)
P(1A) - C(12A) - C(13A) - C(14A)	-169.6(2)
C(12A) - C(13A) - C(14A) - C(15A)	0.8(4)
C(13A) - C(14A) - C(15A) - C(16A)	-0.5(4)
C(14A) - C(15A) - C(16A) - C(17A)	-0.2(4)
C(15A) - C(16A) - C(17A) - C(12A)	0.6(4)
C(13A) - C(12A) - C(17A) - C(16A)	-0.2(4)
P(1A) - C(12A) - C(17A) - C(16A)	168.79(19)
C(12A) - P(1A) - C(18A) - C(19A)	-141.3(2)
C(11A) - P(1A) - C(18A) - C(19A)	113.5(2)
Ru(1A) - P(1A) - C(18A) - C(19A)	-14.0(2)
C(12A) - P(1A) - C(18A) - C(23A)	44.0(2)
C(11A) - P(1A) - C(18A) - C(23A)	-61.2(2)
Ru(1A) - P(1A) - C(18A) - C(23A)	171.36(16)
C(23A) - C(18A) - C(19A) - C(20A)	-0.6(4)
P(1A) - C(18A) - C(19A) - C(20A)	-175.38(19)
C(18A) - C(19A) - C(20A) - C(21A)	0.6(4)
C(19A) - C(20A) - C(21A) - C(22A)	-0.2(4)
C(20A) - C(21A) - C(22A) - C(23A)	-0.2(4)
C(21A) - C(22A) - C(23A) - C(18A)	0.3(4)
C(19A) - C(18A) - C(23A) - C(22A)	0.1(4)
P(1A) - C(18A) - C(23A) - C(22A)	174.86(19)
C(9A) - P(2A) - C(24A) - C(25A)	0.6(2)
C(30A) - P(2A) - C(24A) - C(25A)	-100.3(2)
Ru(1A) - P(2A) - C(24A) - C(25A)	130.99(19)
C(9A) - P(2A) - C(24A) - C(29A)	176.57(18)
C(30A) - P(2A) - C(24A) - C(29A)	75.7(2)
Ru(1A) - P(2A) - C(24A) - C(29A)	-53.02(19)
C(29A) - C(24A) - C(25A) - C(26A)	0.5(4)
P(2A) - C(24A) - C(25A) - C(26A)	176.4(2)
C(24A) - C(25A) - C(26A) - C(27A)	-0.9(4)
C(25A) - C(26A) - C(27A) - C(28A)	0.5(4)
C(26A) - C(27A) - C(28A) - C(29A)	0.3(4)
C(27A) - C(28A) - C(29A) - C(24A)	-0.6(4)
C(25A) - C(24A) - C(29A) - C(28A)	0.3(4)
P(2A) - C(24A) - C(29A) - C(28A)	-176.02(19)
C(24A) - P(2A) - C(30A) - C(31A)	-135.9(2)
C(9A) - P(2A) - C(30A) - C(31A)	118.2(2)
Ru(1A) - P(2A) - C(30A) - C(31A)	-7.9(2)
C(24A) - P(2A) - C(30A) - C(35A)	45.8(2)
C(9A) - P(2A) - C(30A) - C(35A)	-60.0(2)
Ru(1A) - P(2A) - C(30A) - C(35A)	173.91(17)
C(35A) - C(30A) - C(31A) - C(32A)	0.8(4)
P(2A) - C(30A) - C(31A) - C(32A)	-177.45(19)

C(30A) - C(31A) - C(32A) - C(33A)	-0.2(4)
C(31A) - C(32A) - C(33A) - C(34A)	0.0(4)
C(32A) - C(33A) - C(34A) - C(35A)	-0.4(4)
C(33A) - C(34A) - C(35A) - C(30A)	1.0(4)
C(31A) - C(30A) - C(35A) - C(34A)	-1.2(4)
P(2A) - C(30A) - C(35A) - C(34A)	177.1(2)

Table 112. Crystal data and structure refinement for Ru(ICy)(dppp)(CO)H_2.**(78)**

Compound	Ru(ICy)(dppp)(CO)H_2.**(78)**
Empirical formula	C43 H52 N2 O P2 Ru
Formula weight	775.88
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.7350(1)Å α = 79.911(1)^o
	b = 12.2780(2)Å β = 84.049(1)^o
	c = 16.9570(3)Å γ = 69.432(1)^o
Volume	1866.32(5) Å^3
Z	2
Density (calculated)	1.381 Mg/m^3
Absorption coefficient	0.542 mm^{-1}
F(000)	812
Crystal size	0.15 x 0.05 x 0.05 mm
Theta range for data collection	3.52 to 27.53 ^{o}.
Index ranges	-12<=h<=12; -15<=k<=15; -21<=l<=22
Reflections collected	34683
Independent reflections	8540 [R(int) = 0.0656]
Reflections observed (>2σ)	6709
Data Completeness	0.992
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.97 and 0.93
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8540 / 2 / 450
Goodness-of-fit on F^2	1.029
Final R indices [I>2σ(I)]	R1 = 0.0398 wR2 = 0.0713
R indices (all data)	R1 = 0.0631 wR2 = 0.0784
Largest diff. peak and hole	0.448 and -0.761 eÅ^{-3}

Table 113. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Ru(ICy)(dppp)(CO)H_2.**(78)**.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	6596(1)	6328(1)	7305(1)	15(1)
P(1)	7351(1)	4422(1)	7947(1)	17(1)
P(2)	4143(1)	6841(1)	7810(1)	16(1)
O(1)	8230(2)	7106(2)	8413(1)	30(1)
N(1)	6171(2)	8941(2)	6497(1)	17(1)
N(2)	6832(2)	7775(2)	5611(1)	17(1)
C(1)	7571(3)	6828(2)	7999(2)	20(1)
C(2)	6455(3)	7787(2)	6417(1)	16(1)
C(3)	6378(3)	9597(2)	5776(2)	22(1)

C(4)	6788(3)	8875(2)	5225(2)	22(1)
C(5)	5643(3)	9476(2)	7231(2)	18(1)
C(6)	6743(3)	9973(2)	7476(2)	25(1)
C(7)	6188(3)	10547(3)	8226(2)	29(1)
C(8)	4683(3)	11511(3)	8102(2)	32(1)
C(9)	3574(3)	11017(2)	7865(2)	27(1)
C(10)	4128(3)	10426(2)	7120(2)	22(1)
C(11)	7201(3)	6750(2)	5182(2)	19(1)
C(12)	5840(3)	6716(2)	4828(2)	24(1)
C(13)	6224(3)	5670(3)	4371(2)	31(1)
C(14)	7448(3)	5661(3)	3737(2)	32(1)
C(15)	8792(3)	5677(3)	4107(2)	31(1)
C(16)	8413(3)	6746(3)	4535(2)	26(1)
C(17)	8803(3)	4046(2)	8657(2)	20(1)
C(18)	8658(3)	3658(3)	9471(2)	30(1)
C(19)	9825(3)	3373(3)	9967(2)	38(1)
C(20)	11154(3)	3460(3)	9651(2)	32(1)
C(21)	11313(3)	3844(2)	8843(2)	27(1)
C(22)	10154(3)	4145(2)	8352(2)	24(1)
C(23)	8173(3)	3252(2)	7314(2)	20(1)
C(24)	7709(3)	3425(2)	6540(2)	25(1)
C(25)	8217(3)	2538(3)	6067(2)	30(1)
C(26)	9226(3)	1470(3)	6353(2)	30(1)
C(27)	9718(3)	1277(2)	7118(2)	30(1)
C(28)	9192(3)	2161(2)	7599(2)	28(1)
C(29)	5989(3)	3830(2)	8513(2)	21(1)
C(30)	4764(3)	4730(2)	8943(2)	22(1)
C(31)	3630(3)	5590(2)	8364(2)	21(1)
C(32)	2670(3)	7445(2)	7085(2)	18(1)
C(33)	2883(3)	8144(2)	6376(2)	20(1)
C(34)	1822(3)	8594(2)	5804(2)	22(1)
C(35)	534(3)	8325(2)	5926(2)	26(1)
C(36)	306(3)	7635(2)	6622(2)	26(1)
C(37)	1353(3)	7202(2)	7204(2)	23(1)
C(38)	3453(3)	7850(2)	8567(2)	19(1)
C(39)	4416(3)	7846(2)	9124(2)	24(1)
C(40)	3941(3)	8556(3)	9721(2)	32(1)
C(41)	2497(3)	9291(3)	9771(2)	33(1)
C(42)	1522(3)	9307(3)	9227(2)	32(1)
C(43)	1991(3)	8589(2)	8636(2)	26(1)

Table 114. Bond lengths [Å] and angles [^{o}] for Ru(ICy)(dppp)(CO)H_2.**(78)**.

Ru(1)-C(1)	1.886(3)	C(16)-H(16A)	0.9900
Ru(1)-C(2)	2.103(3)	C(16)-H(16B)	0.9900
Ru(1)-P(1)	2.2947(7)	C(17)-C(18)	1.389(4)
Ru(1)-P(2)	2.3537(7)	C(17)-C(22)	1.400(4)
Ru(1)-H(1)	1.607(10)	C(18)-C(19)	1.391(4)
Ru(1)-H(2)	1.592(10)	C(18)-H(18)	0.9500
P(1)-C(17)	1.834(3)	C(19)-C(20)	1.380(4)
P(1)-C(29)	1.837(3)	C(19)-H(19)	0.9500
P(1)-C(23)	1.847(3)	C(20)-C(21)	1.380(4)
P(2)-C(32)	1.848(3)	C(20)-H(20)	0.9500
P(2)-C(31)	1.851(3)	C(21)-C(22)	1.377(4)
P(2)-C(38)	1.853(3)	C(21)-H(21)	0.9500

O(1)-C(1)	1.162(3)	C(22)-H(22)	0.9500
N(1)-C(2)	1.374(3)	C(23)-C(24)	1.388(4)
N(1)-C(3)	1.379(3)	C(23)-C(28)	1.397(4)
N(1)-C(5)	1.470(3)	C(24)-C(25)	1.386(4)
N(2)-C(2)	1.379(3)	C(24)-H(24)	0.9500
N(2)-C(4)	1.381(3)	C(25)-C(26)	1.375(4)
N(2)-C(11)	1.480(3)	C(25)-H(25)	0.9500
C(3)-C(4)	1.336(4)	C(26)-C(27)	1.381(4)
C(3)-H(3)	0.9500	C(26)-H(26)	0.9500
C(4)-H(4)	0.9500	C(27)-C(28)	1.392(4)
C(5)-C(6)	1.527(3)	C(27)-H(27)	0.9500
C(5)-C(10)	1.531(3)	C(28)-H(28)	0.9500
C(5)-H(5)	1.0000	C(29)-C(30)	1.533(4)
C(6)-C(7)	1.520(4)	C(29)-H(29A)	0.9900
C(6)-H(6A)	0.9900	C(29)-H(29B)	0.9900
C(6)-H(6B)	0.9900	C(30)-C(31)	1.530(4)
C(7)-C(8)	1.533(4)	C(30)-H(30A)	0.9900
C(7)-H(7A)	0.9900	C(30)-H(30B)	0.9900
C(7)-H(7B)	0.9900	C(31)-H(31A)	0.9900
C(8)-C(9)	1.527(4)	C(31)-H(31B)	0.9900
C(8)-H(8A)	0.9900	C(32)-C(33)	1.392(4)
C(8)-H(8B)	0.9900	C(32)-C(37)	1.403(4)
C(9)-C(10)	1.523(4)	C(33)-C(34)	1.390(4)
C(9)-H(9A)	0.9900	C(33)-H(33)	0.9500
C(9)-H(9B)	0.9900	C(34)-C(35)	1.392(4)
C(10)-H(10A)	0.9900	C(34)-H(34)	0.9500
C(10)-H(10B)	0.9900	C(35)-C(36)	1.373(4)
C(11)-C(16)	1.525(4)	C(35)-H(35)	0.9500
C(11)-C(12)	1.527(3)	C(36)-C(37)	1.392(4)
C(11)-H(11)	1.0000	C(36)-H(36)	0.9500
C(12)-C(13)	1.530(4)	C(37)-H(37)	0.9500
C(12)-H(12A)	0.9900	C(38)-C(43)	1.400(4)
C(12)-H(12B)	0.9900	C(38)-C(39)	1.395(4)
C(13)-C(14)	1.519(4)	C(39)-C(40)	1.389(4)
C(13)-H(13A)	0.9900	C(39)-H(39)	0.9500
C(13)-H(13B)	0.9900	C(40)-C(41)	1.381(4)
C(14)-C(15)	1.516(4)	C(40)-H(40)	0.9500
C(14)-H(14A)	0.9900	C(41)-C(42)	1.384(4)
C(14)-H(14B)	0.9900	C(41)-H(41)	0.9500
C(15)-C(16)	1.526(4)	C(42)-C(43)	1.387(4)
C(15)-H(15A)	0.9900	C(42)-H(42)	0.9500
C(15)-H(15B)	0.9900	C(43)-H(43)	0.9500
C(1)-Ru(1)-C(2)	92.76(10)	C(14)-C(15)-C(16)	110.8(2)
C(1)-Ru(1)-P(1)	93.32(8)	C(14)-C(15)-H(15A)	109.5
C(2)-Ru(1)-P(1)	159.81(7)	C(16)-C(15)-H(15A)	109.5
C(1)-Ru(1)-P(2)	105.17(8)	C(14)-C(15)-H(15B)	109.5
C(2)-Ru(1)-P(2)	100.51(7)	C(16)-C(15)-H(15B)	109.5
P(1)-Ru(1)-P(2)	96.44(2)	H(15A)-C(15)-H(15B)	108.1
C(1)-Ru(1)-H(1)	176.1(10)	C(11)-C(16)-C(15)	110.5(2)
C(2)-Ru(1)-H(1)	87.1(10)	C(11)-C(16)-H(16A)	109.5
P(1)-Ru(1)-H(1)	85.5(10)	C(15)-C(16)-H(16A)	109.5
P(2)-Ru(1)-H(1)	78.7(10)	C(11)-C(16)-H(16B)	109.5
C(1)-Ru(1)-H(2)	88.8(10)	C(15)-C(16)-H(16B)	109.5
C(2)-Ru(1)-H(2)	80.8(10)	H(16A)-C(16)-H(16B)	108.1

P(1)-Ru(1)-H(2)	80.1(10)	C(18)-C(17)-C(22)	118.1(2)
P(2)-Ru(1)-H(2)	165.8(10)	C(18)-C(17)-P(1)	124.5(2)
H(1)-Ru(1)-H(2)	87.3(14)	C(22)-C(17)-P(1)	117.5(2)
C(17)-P(1)-C(29)	103.47(12)	C(17)-C(18)-C(19)	120.8(3)
C(17)-P(1)-C(23)	100.46(12)	C(17)-C(18)-H(18)	119.6
C(29)-P(1)-C(23)	97.82(12)	C(19)-C(18)-H(18)	119.6
C(17)-P(1)-Ru(1)	115.59(9)	C(20)-C(19)-C(18)	120.1(3)
C(29)-P(1)-Ru(1)	119.34(9)	C(20)-C(19)-H(19)	119.9
C(23)-P(1)-Ru(1)	117.03(9)	C(18)-C(19)-H(19)	119.9
C(32)-P(2)-C(31)	99.40(12)	C(21)-C(20)-C(19)	119.6(3)
C(32)-P(2)-C(38)	101.80(11)	C(21)-C(20)-H(20)	120.2
C(31)-P(2)-C(38)	98.17(12)	C(19)-C(20)-H(20)	120.2
C(32)-P(2)-Ru(1)	118.17(8)	C(22)-C(21)-C(20)	120.4(3)
C(31)-P(2)-Ru(1)	114.46(9)	C(22)-C(21)-H(21)	119.8
C(38)-P(2)-Ru(1)	121.00(8)	C(20)-C(21)-H(21)	119.8
C(2)-N(1)-C(3)	111.5(2)	C(21)-C(22)-C(17)	120.9(3)
C(2)-N(1)-C(5)	126.6(2)	C(21)-C(22)-H(22)	119.5
C(3)-N(1)-C(5)	121.8(2)	C(17)-C(22)-H(22)	119.5
C(2)-N(2)-C(4)	111.3(2)	C(24)-C(23)-C(28)	118.1(2)
C(2)-N(2)-C(11)	126.2(2)	C(24)-C(23)-P(1)	119.4(2)
C(4)-N(2)-C(11)	122.5(2)	C(28)-C(23)-P(1)	122.4(2)
O(1)-C(1)-Ru(1)	177.0(2)	C(25)-C(24)-C(23)	121.2(3)
N(1)-C(2)-N(2)	102.8(2)	C(25)-C(24)-H(24)	119.4
N(1)-C(2)-Ru(1)	129.53(17)	C(23)-C(24)-H(24)	119.4
N(2)-C(2)-Ru(1)	127.14(18)	C(26)-C(25)-C(24)	120.1(3)
C(4)-C(3)-N(1)	107.2(2)	C(26)-C(25)-H(25)	119.9
C(4)-C(3)-H(3)	126.4	C(24)-C(25)-H(25)	119.9
N(1)-C(3)-H(3)	126.4	C(25)-C(26)-C(27)	119.8(3)
C(3)-C(4)-N(2)	107.1(2)	C(25)-C(26)-H(26)	120.1
C(3)-C(4)-H(4)	126.5	C(27)-C(26)-H(26)	120.1
N(2)-C(4)-H(4)	126.5	C(26)-C(27)-C(28)	120.2(3)
N(1)-C(5)-C(6)	110.9(2)	C(26)-C(27)-H(27)	119.9
N(1)-C(5)-C(10)	110.6(2)	C(28)-C(27)-H(27)	119.9
C(6)-C(5)-C(10)	111.1(2)	C(27)-C(28)-C(23)	120.6(3)
N(1)-C(5)-H(5)	108.0	C(27)-C(28)-H(28)	119.7
C(6)-C(5)-H(5)	108.0	C(23)-C(28)-H(28)	119.7
C(10)-C(5)-H(5)	108.0	C(30)-C(29)-P(1)	113.93(18)
C(7)-C(6)-C(5)	111.1(2)	C(30)-C(29)-H(29A)	108.8
C(7)-C(6)-H(6A)	109.4	P(1)-C(29)-H(29A)	108.8
C(5)-C(6)-H(6A)	109.4	C(30)-C(29)-H(29B)	108.8
C(7)-C(6)-H(6B)	109.4	P(1)-C(29)-H(29B)	108.8
C(5)-C(6)-H(6B)	109.4	H(29A)-C(29)-H(29B)	107.7
H(6A)-C(6)-H(6B)	108.0	C(31)-C(30)-C(29)	112.0(2)
C(6)-C(7)-C(8)	110.8(2)	C(31)-C(30)-H(30A)	109.2
C(6)-C(7)-H(7A)	109.5	C(29)-C(30)-H(30A)	109.2
C(8)-C(7)-H(7A)	109.5	C(31)-C(30)-H(30B)	109.2
C(6)-C(7)-H(7B)	109.5	C(29)-C(30)-H(30B)	109.2
C(8)-C(7)-H(7B)	109.5	H(30A)-C(30)-H(30B)	107.9
H(7A)-C(7)-H(7B)	108.1	C(30)-C(31)-P(2)	115.12(18)
C(9)-C(8)-C(7)	110.9(2)	C(30)-C(31)-H(31A)	108.5
C(9)-C(8)-H(8A)	109.4	P(2)-C(31)-H(31A)	108.5
C(7)-C(8)-H(8A)	109.4	C(30)-C(31)-H(31B)	108.5
C(9)-C(8)-H(8B)	109.4	P(2)-C(31)-H(31B)	108.5
C(7)-C(8)-H(8B)	109.4	H(31A)-C(31)-H(31B)	107.5
H(8A)-C(8)-H(8B)	108.0	C(33)-C(32)-C(37)	117.9(2)

C(10)-C(9)-C(8)	110.9(2)	C(33)-C(32)-P(2)	119.09(19)
C(10)-C(9)-H(9A)	109.5	C(37)-C(32)-P(2)	123.0(2)
C(8)-C(9)-H(9A)	109.5	C(34)-C(33)-C(32)	121.2(2)
C(10)-C(9)-H(9B)	109.5	C(34)-C(33)-H(33)	119.4
C(8)-C(9)-H(9B)	109.5	C(32)-C(33)-H(33)	119.4
H(9A)-C(9)-H(9B)	108.0	C(33)-C(34)-C(35)	120.0(3)
C(9)-C(10)-C(5)	111.6(2)	C(33)-C(34)-H(34)	120.0
C(9)-C(10)-H(10A)	109.3	C(35)-C(34)-H(34)	120.0
C(5)-C(10)-H(10A)	109.3	C(36)-C(35)-C(34)	119.6(2)
C(9)-C(10)-H(10B)	109.3	C(36)-C(35)-H(35)	120.2
C(5)-C(10)-H(10B)	109.3	C(34)-C(35)-H(35)	120.2
H(10A)-C(10)-H(10B)	108.0	C(35)-C(36)-C(37)	120.6(2)
N(2)-C(11)-C(16)	111.2(2)	C(35)-C(36)-H(36)	119.7
N(2)-C(11)-C(12)	111.0(2)	C(37)-C(36)-H(36)	119.7
C(16)-C(11)-C(12)	111.0(2)	C(36)-C(37)-C(32)	120.7(3)
N(2)-C(11)-H(11)	107.8	C(36)-C(37)-H(37)	119.6
C(16)-C(11)-H(11)	107.8	C(32)-C(37)-H(37)	119.6
C(12)-C(11)-H(11)	107.8	C(43)-C(38)-C(39)	117.6(2)
C(11)-C(12)-C(13)	111.1(2)	C(43)-C(38)-P(2)	123.4(2)
C(11)-C(12)-H(12A)	109.4	C(39)-C(38)-P(2)	118.9(2)
C(13)-C(12)-H(12A)	109.4	C(40)-C(39)-C(38)	121.1(3)
C(11)-C(12)-H(12B)	109.4	C(40)-C(39)-H(39)	119.4
C(13)-C(12)-H(12B)	109.4	C(38)-C(39)-H(39)	119.4
H(12A)-C(12)-H(12B)	108.0	C(41)-C(40)-C(39)	120.3(3)
C(14)-C(13)-C(12)	111.7(2)	C(41)-C(40)-H(40)	119.8
C(14)-C(13)-H(13A)	109.3	C(39)-C(40)-H(40)	119.8
C(12)-C(13)-H(13A)	109.3	C(40)-C(41)-C(42)	119.6(3)
C(14)-C(13)-H(13B)	109.3	C(40)-C(41)-H(41)	120.2
C(12)-C(13)-H(13B)	109.3	C(42)-C(41)-H(41)	120.2
H(13A)-C(13)-H(13B)	107.9	C(41)-C(42)-C(43)	120.2(3)
C(15)-C(14)-C(13)	110.7(2)	C(41)-C(42)-H(42)	119.9
C(15)-C(14)-H(14A)	109.5	C(43)-C(42)-H(42)	119.9
C(13)-C(14)-H(14A)	109.5	C(38)-C(43)-C(42)	121.1(3)
C(15)-C(14)-H(14B)	109.5	C(38)-C(43)-H(43)	119.4
C(13)-C(14)-H(14B)	109.5	C(42)-C(43)-H(43)	119.4
H(14A)-C(14)-H(14B)	108.1		

Table 115. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Ru(ICy)(dppp)(CO)H_2$.**(78)**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	15(1)	16(1)	14(1)	-1(1)	-1(1)	-7(1)
P(1)	18(1)	18(1)	16(1)	-1(1)	-2(1)	-8(1)
P(2)	15(1)	18(1)	16(1)	-2(1)	0(1)	-7(1)
O(1)	35(1)	35(1)	27(1)	-4(1)	-11(1)	-18(1)
N(1)	20(1)	18(1)	16(1)	0(1)	-1(1)	-9(1)
N(2)	18(1)	18(1)	17(1)	0(1)	-2(1)	-8(1)
C(1)	20(1)	18(1)	20(1)	1(1)	0(1)	-6(1)
C(2)	13(1)	22(1)	15(1)	-3(1)	-2(1)	-9(1)
C(3)	24(1)	18(1)	21(1)	4(1)	-1(1)	-9(1)
C(4)	24(1)	22(2)	20(1)	2(1)	0(1)	-10(1)
C(5)	21(1)	17(1)	17(1)	-2(1)	1(1)	-9(1)

C(6)	24(1)	27(2)	28(2)	-6(1)	-2(1)	-11(1)
C(7)	32(2)	32(2)	30(2)	-9(1)	-7(1)	-13(1)
C(8)	39(2)	25(2)	33(2)	-13(1)	-3(1)	-8(1)
C(9)	26(2)	24(2)	30(2)	-8(1)	2(1)	-7(1)
C(10)	20(1)	23(2)	24(2)	-4(1)	-2(1)	-8(1)
C(11)	20(1)	18(1)	17(1)	-3(1)	-1(1)	-5(1)
C(12)	20(1)	26(2)	25(2)	-7(1)	-1(1)	-7(1)
C(13)	35(2)	31(2)	31(2)	-8(1)	-6(1)	-14(1)
C(14)	40(2)	33(2)	23(2)	-13(1)	-4(1)	-6(1)
C(15)	28(2)	36(2)	25(2)	-13(1)	6(1)	-5(1)
C(16)	24(1)	31(2)	22(2)	-6(1)	3(1)	-10(1)
C(17)	21(1)	17(1)	22(1)	-1(1)	-4(1)	-6(1)
C(18)	25(2)	41(2)	22(2)	1(1)	-1(1)	-11(1)
C(19)	35(2)	57(2)	19(2)	3(2)	-8(1)	-15(2)
C(20)	26(2)	42(2)	29(2)	-1(1)	-12(1)	-11(1)
C(21)	23(1)	28(2)	31(2)	1(1)	-5(1)	-13(1)
C(22)	26(1)	25(2)	21(1)	2(1)	-3(1)	-11(1)
C(23)	18(1)	17(1)	25(2)	-2(1)	0(1)	-8(1)
C(24)	28(2)	20(2)	26(2)	-4(1)	-3(1)	-7(1)
C(25)	35(2)	29(2)	26(2)	-8(1)	-3(1)	-9(1)
C(26)	31(2)	22(2)	39(2)	-13(1)	10(1)	-11(1)
C(27)	26(2)	18(2)	42(2)	-2(1)	-1(1)	-3(1)
C(28)	31(2)	22(2)	29(2)	-2(1)	-5(1)	-9(1)
C(29)	23(1)	18(1)	23(2)	2(1)	-3(1)	-10(1)
C(30)	24(1)	24(2)	19(1)	2(1)	1(1)	-12(1)
C(31)	18(1)	22(1)	22(1)	-1(1)	1(1)	-9(1)
C(32)	16(1)	18(1)	19(1)	-6(1)	-1(1)	-4(1)
C(33)	15(1)	24(2)	24(2)	-5(1)	1(1)	-9(1)
C(34)	22(1)	25(2)	20(1)	-1(1)	-2(1)	-9(1)
C(35)	19(1)	31(2)	27(2)	-7(1)	-7(1)	-6(1)
C(36)	15(1)	31(2)	33(2)	-6(1)	-2(1)	-10(1)
C(37)	19(1)	27(2)	25(2)	0(1)	0(1)	-11(1)
C(38)	22(1)	21(1)	16(1)	-1(1)	2(1)	-11(1)
C(39)	26(1)	27(2)	21(1)	-3(1)	1(1)	-10(1)
C(40)	38(2)	39(2)	22(2)	-7(1)	-1(1)	-18(2)
C(41)	41(2)	35(2)	23(2)	-14(1)	8(1)	-13(2)
C(42)	27(2)	32(2)	32(2)	-10(1)	9(1)	-5(1)
C(43)	22(1)	29(2)	24(2)	-6(1)	2(1)	-7(1)

Table 116. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(ICy)(dppp)(CO)H_2.**(78)**.

Atom	x	y	z	U(eq)
H(1)	5870(30)	5860(20)	6687(13)	31(8)
H(2)	8123(18)	5810(20)	6827(15)	33(8)
H(3)	6252	10411	5688	26
H(4)	7007	9079	4672	26
H(5)	5545	8846	7672	22
H(6A)	7694	9331	7578	30
H(6B)	6909	10561	7032	30
H(7A)	6898	10894	8357	35
H(7B)	6111	9944	8682	35
H(8A)	4325	11851	8603	38
H(8B)	4779	12147	7676	38

H(9A)	3402	10437	8314	32
H(9B)	2628	11662	7760	32
H(10A)	4185	11027	6657	26
H(10B)	3422	10067	7000	26
H(11)	7575	6022	5581	22
H(12A)	5405	7456	4460	28
H(12B)	5100	6656	5265	28
H(13A)	6532	4929	4754	37
H(13B)	5340	5707	4111	37
H(14A)	7709	4949	3477	39
H(14B)	7104	6358	3320	39
H(15A)	9565	5696	3682	37
H(15B)	9181	4950	4494	37
H(16A)	9298	6732	4782	31
H(16B)	8084	7474	4142	31
H(18)	7751	3585	9692	36
H(19)	9707	3119	10524	46
H(20)	11955	3256	9988	39
H(21)	12228	3902	8624	32
H(22)	10273	4423	7799	28
H(24)	7030	4166	6331	30
H(25)	7869	2668	5544	36
H(26)	9583	865	6026	36
H(27)	10416	541	7316	36
H(28)	9528	2020	8126	33
H(29A)	5541	3529	8140	25
H(29B)	6499	3157	8916	25
H(30A)	4267	4309	9362	26
H(30B)	5202	5176	9212	26
H(31A)	2692	5907	8672	25
H(31B)	3457	5149	7971	25
H(33)	3768	8318	6282	24
H(34)	1976	9085	5329	27
H(35)	-183	8616	5530	31
H(36)	-574	7453	6707	31
H(37)	1173	6736	7686	28
H(39)	5413	7348	9094	29
H(40)	4612	8537	10096	38
H(41)	2176	9782	10177	39
H(42)	528	9812	9259	38
H(43)	1307	8599	8271	31

Table 117. Crystal data and structure refinement for Ru(ICy)(dppp)(CO)HF **(79)**.

Compound	Ru(ICy)(dppp)(CO)HF **(79)**
Empirical formula	C44.33 H54 F N2 O P2 Ru
Formula weight	812.91
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Hexagonal
Space group	P61
Unit cell dimensions	a = 40.3130(2)Å α = 90°
	b = 40.3130(2)Å β = 90°
	c = 14.5800(1)Å γ = 120°
Volume	20520.0(2) $Å^3$
Z	18
Density (calculated)	1.184 Mg/m^3
Absorption coefficient	0.450 mm^{-1}
F(000)	7650
Crystal size	0.20 x 0.08 x 0.05 mm
Theta range for data collection	3.54 to 23.25°
Index ranges	-44<=h<=44; -44<=k<=44; -16<=l<=16
Reflections collected	221677
Independent reflections	19537 [R(int) = 0.1287]
Reflections observed (>2σ)	15208
Data Completeness	0.995
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.98 and 0.93
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19537 / 13 / 1387
Goodness-of-fit on F^2	1.025
Final R indices [I>2σ(I)]	R1 = 0.0535 wR2 = 0.1200
R indices (all data)	R1 = 0.0805 wR2 = 0.1332
Absolute structure parameter	-0.02(3)
Largest diff. peak and hole	0.984 and -0.327 $eÅ^{-3}$

Table 118. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ru(ICy)(dppp)(CO)HF **(79)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	3526(1)	-1794(1)	148(1)	32(1)
Ru(2)	3702(1)	1257(1)	-1446(1)	29(1)
Ru(3)	2847(1)	-285(1)	-6459(1)	30(1)
P(1)	3317(1)	-2367(1)	-639(1)	43(1)
P(2)	3798(1)	-1420(1)	-1227(1)	36(1)
P(3)	4058(1)	1347(1)	-2851(1)	34(1)
P(4)	3121(1)	949(1)	-2238(1)	39(1)
P(5)	3406(1)	20(1)	-7331(1)	31(1)
P(6)	2453(1)	-393(1)	-7802(1)	36(1)
F(1)	3011(1)	-1846(1)	-379(2)	39(1)
F(2)	3702(1)	1754(1)	-1927(3)	35(1)
F(3)	2854(1)	-773(1)	-6956(2)	32(1)
O(1)	4207(2)	-1771(2)	1015(4)	55(2)
O(2)	3621(1)	541(1)	-651(3)	40(1)
O(3)	2922(2)	424(2)	-5635(4)	54(2)

N(1)	3874(2)	-1004(2)	1245(4)	29(1)
N(2)	3279(2)	-1385(2)	1562(4)	33(1)
N(3)	4512(2)	1605(2)	-448(4)	34(1)
N(4)	4221(2)	1913(2)	-111(4)	33(1)
N(5)	2070(2)	-654(2)	-5305(4)	43(2)
N(6)	2397(2)	-930(2)	-5049(4)	34(1)
C(1)	3942(2)	-1775(2)	658(5)	41(2)
C(2)	3578(2)	-1352(2)	1039(5)	30(2)
C(3)	3769(2)	-823(2)	1902(5)	35(2)
C(4)	3392(2)	-1060(2)	2091(4)	34(2)
C(5)	4265(2)	-824(2)	897(5)	34(2)
C(6)	4400(2)	-414(2)	583(5)	36(2)
C(7)	4803(2)	-231(2)	209(6)	45(2)
C(8)	5082(2)	-229(2)	907(6)	49(2)
C(9)	4947(2)	-641(2)	1233(6)	49(2)
C(10)	4539(2)	-832(2)	1615(5)	41(2)
C(11)	2897(2)	-1725(2)	1646(5)	35(2)
C(12)	2890(2)	-1947(2)	2512(5)	57(2)
C(13)	2498(3)	-2305(3)	2648(7)	82(3)
C(14)	2185(3)	-2207(3)	2590(6)	83(4)
C(15)	2201(2)	-1994(3)	1728(7)	71(3)
C(16)	2592(2)	-1624(2)	1635(6)	52(2)
C(17)	3182(3)	-2377(2)	-1850(5)	60(3)
C(18)	3456(2)	-2044(2)	-2454(5)	53(2)
C(19)	3483(2)	-1664(2)	-2215(5)	45(2)
C(20)	3629(3)	-2573(2)	-581(7)	58(2)
C(21)	3702(3)	-2663(3)	291(9)	77(3)
C(22)	3933(4)	-2825(3)	420(12)	113(5)
C(23)	4109(4)	-2875(4)	-327(17)	133(7)
C(24)	4016(5)	-2793(4)	-1212(14)	140(7)
C(25)	3790(3)	-2646(3)	-1290(10)	107(5)
C(26)	2854(2)	-2774(2)	-274(6)	46(2)
C(27)	2598(2)	-2723(2)	213(6)	48(2)
C(28)	2245(2)	-3035(2)	461(6)	61(3)
C(29)	2153(3)	-3397(2)	220(7)	67(3)
C(30)	2408(3)	-3455(3)	-263(7)	76(3)
C(31)	2759(3)	-3145(2)	-522(7)	67(3)
C(32)	3813(2)	-952(2)	-1292(5)	38(2)
C(33)	4099(2)	-626(2)	-1714(5)	46(2)
C(34)	4081(3)	-292(2)	-1699(5)	55(2)
C(35)	3783(3)	-281(2)	-1275(6)	56(2)
C(36)	3503(2)	-603(2)	-860(5)	44(2)
C(37)	3512(2)	-935(2)	-870(5)	41(2)
C(38)	4269(2)	-1310(2)	-1684(5)	40(2)
C(39)	4530(2)	-1345(2)	-1137(6)	51(2)
C(40)	4879(2)	-1278(2)	-1467(7)	61(2)
C(41)	4982(3)	-1163(2)	-2360(8)	65(3)
C(42)	4735(3)	-1126(2)	-2920(7)	66(3)
C(43)	4376(2)	-1200(2)	-2589(6)	52(2)
C(44)	3661(2)	829(2)	-973(5)	36(2)
C(45)	4176(2)	1608(2)	-618(4)	30(2)
C(46)	4746(2)	1898(2)	141(5)	40(2)
C(47)	4564(2)	2090(2)	349(5)	41(2)
C(48)	4608(2)	1325(2)	-799(5)	37(2)
C(49)	5017(2)	1512(2)	-1150(6)	47(2)

C(50)	5082(2)	1207(3)	-1618(7)	62(2)
C(51)	5021(3)	894(3)	-923(7)	70(3)
C(52)	4616(3)	715(2)	-518(7)	62(2)
C(53)	4541(2)	1022(2)	-81(5)	46(2)
C(54)	3928(2)	2026(2)	3(4)	35(2)
C(55)	3756(3)	1926(3)	961(6)	55(2)
C(56)	3454(3)	2044(3)	1094(6)	67(3)
C(57)	3611(3)	2456(3)	863(6)	66(3)
C(58)	3777(3)	2545(3)	-83(5)	57(2)
C(59)	4090(2)	2449(2)	-198(5)	49(2)
C(60)	3120(2)	1105(2)	-3423(5)	47(2)
C(61)	3437(2)	1136(2)	-4057(5)	44(2)
C(62)	3839(2)	1470(2)	-3810(5)	42(2)
C(63)	2878(2)	430(2)	-2315(6)	48(2)
C(64)	2758(2)	226(2)	-1494(6)	52(2)
C(65)	2564(3)	-170(2)	-1497(7)	72(3)
C(66)	2498(3)	-372(2)	-2336(8)	74(3)
C(67)	2621(3)	-169(2)	-3156(8)	78(3)
C(68)	2809(2)	229(2)	-3143(6)	62(2)
C(69)	2740(2)	1015(2)	-1776(6)	53(2)
C(70)	2811(3)	1311(3)	-1164(6)	56(2)
C(71)	2536(3)	1388(3)	-832(7)	69(3)
C(72)	2179(5)	1175(5)	-1107(10)	108(5)
C(73)	2075(3)	873(5)	-1700(12)	119(6)
C(74)	2353(3)	785(3)	-2084(8)	83(3)
C(75)	4087(2)	948(2)	-3381(5)	36(2)
C(76)	4244(2)	972(2)	-4259(5)	46(2)
C(77)	4214(2)	654(2)	-4680(5)	49(2)
C(78)	4020(2)	304(2)	-4266(6)	51(2)
C(79)	3862(2)	270(2)	-3397(5)	48(2)
C(80)	3896(2)	593(2)	-2971(5)	39(2)
C(81)	4541(2)	1767(2)	-2884(5)	38(2)
C(82)	4866(2)	1789(2)	-3293(6)	50(2)
C(83)	5210(2)	2132(2)	-3319(6)	55(2)
C(84)	5239(2)	2453(2)	-2910(6)	60(3)
C(85)	4921(2)	2432(2)	-2476(6)	53(2)
C(86)	4580(2)	2099(2)	-2473(5)	41(2)
C(87)	2886(2)	147(2)	-5986(5)	39(2)
C(88)	2399(2)	-642(2)	-5554(4)	32(2)
C(89)	1876(2)	-935(2)	-4654(5)	46(2)
C(90)	2072(2)	-1112(2)	-4513(5)	40(2)
C(91)	1934(2)	-394(2)	-5626(6)	52(2)
C(92)	1515(3)	-612(3)	-5884(7)	76(3)
C(93)	1400(4)	-346(4)	-6291(10)	112(4)
C(94)	1461(4)	-38(5)	-5656(11)	130(6)
C(95)	1899(4)	195(4)	-5341(9)	112(5)
C(96)	2012(3)	-87(3)	-4945(6)	67(3)
C(97)	2709(2)	-1018(2)	-5006(5)	36(2)
C(98)	2919(2)	-889(2)	-4090(5)	53(2)
C(99)	3243(3)	-973(3)	-4027(6)	65(3)
C(100)	3101(3)	-1395(3)	-4233(5)	65(3)
C(101)	2900(3)	-1512(2)	-5144(5)	54(2)
C(102)	2565(2)	-1439(2)	-5173(5)	47(2)
C(103)	3370(2)	-164(2)	-8509(5)	34(2)
C(104)	3042(2)	-194(2)	-9093(5)	36(2)

C(105)	2654(2)	-516(2)	-8786(5)	37(2)
C(106)	3651(2)	543(2)	-7453(5)	33(2)
C(107)	3763(2)	757(2)	-6651(5)	42(2)
C(108)	3971(3)	1153(2)	-6686(6)	64(3)
C(109)	4063(3)	1336(2)	-7522(6)	63(3)
C(110)	3938(3)	1126(2)	-8303(6)	59(2)
C(111)	3732(2)	723(2)	-8289(5)	45(2)
C(112)	3803(2)	-37(2)	-6933(5)	33(2)
C(113)	3741(2)	-328(2)	-6291(5)	40(2)
C(114)	4038(2)	-385(2)	-6019(5)	44(2)
C(115)	4399(2)	-156(2)	-6364(6)	51(2)
C(116)	4470(2)	133(2)	-6986(6)	53(2)
C(117)	4185(2)	193(2)	-7255(6)	44(2)
C(118)	2390(2)	-10(3)	-8305(5)	52(2)
C(119)	2565(3)	345(3)	-7896(6)	72(3)
C(120)	2552(4)	647(3)	-8315(9)	107(4)
C(121)	2388(5)	615(4)	-9138(9)	113(5)
C(122)	2214(4)	257(4)	-9537(7)	92(4)
C(123)	2214(3)	-55(3)	-9140(6)	70(3)
C(124)	1980(2)	-819(2)	-7776(5)	44(2)
C(125)	1641(2)	-851(3)	-8065(6)	72(3)
C(126)	1289(3)	-1210(4)	-8009(8)	91(4)
C(127)	1289(3)	-1523(3)	-7676(7)	87(3)
C(128)	1616(3)	-1503(3)	-7405(7)	69(3)
C(129)	1963(2)	-1146(2)	-7431(5)	49(2)
C(201)	6129(5)	1431(4)	-953(11)	101(6)
C(202)	6164(11)	1803(6)	-657(11)	246(16)
C(203)	6126(4)	1985(3)	-1538(9)	80(4)
C(204)	6167(5)	2357(4)	-1241(10)	104(6)
C(205)	6133(7)	2543(5)	-2092(11)	146(8)
C(206)	6190(9)	2927(5)	-1830(17)	206(13)

Table 119. Bond lengths [Å] and angles [°] for Ru(ICy)(dppp)(CO)HF **(79)**.

Ru(1)-C(1)	1.801(9)	Ru(1)-F(1)	2.121(4)
Ru(1)-C(2)	2.130(7)	Ru(1)-P(1)	2.328(2)
Ru(1)-P(2)	2.4177(19)	Ru(2)-C(44)	1.791(8)
Ru(2)-C(45)	2.098(7)	Ru(2)-F(2)	2.120(3)
Ru(2)-P(4)	2.334(2)	Ru(2)-P(3)	2.4229(19)
Ru(3)-C(87)	1.805(8)	Ru(3)-F(3)	2.110(3)
Ru(3)-C(88)	2.113(7)	Ru(3)-P(5)	2.3314(19)
Ru(3)-P(6)	2.4188(19)	P(1)-C(20)	1.818(10)
P(1)-C(17)	1.842(8)	P(1)-C(26)	1.843(8)
P(2)-C(38)	1.845(8)	P(2)-C(19)	1.846(7)
P(2)-C(32)	1.857(7)	P(3)-C(81)	1.834(7)
P(3)-C(75)	1.840(7)	P(3)-C(62)	1.851(7)
P(4)-C(69)	1.813(9)	P(4)-C(63)	1.818(8)
P(4)-C(60)	1.841(7)	P(5)-C(112)	1.826(7)
P(5)-C(106)	1.834(7)	P(5)-C(103)	1.847(7)
P(6)-C(124)	1.821(8)	P(6)-C(105)	1.833(7)
P(6)-C(118)	1.836(8)	O(1)-C(1)	1.182(9)
O(2)-C(44)	1.184(8)	O(3)-C(87)	1.169(8)
N(1)-C(2)	1.345(8)	N(1)-C(3)	1.393(8)
N(1)-C(5)	1.458(8)	N(2)-C(2)	1.374(8)
N(2)-C(4)	1.386(8)	N(2)-C(11)	1.469(8)

N(3)-C(45)	1.382(8)	N(3)-C(46)	1.382(9)
N(3)-C(48)	1.459(8)	N(4)-C(45)	1.367(8)
N(4)-C(47)	1.373(9)	N(4)-C(54)	1.472(8)
N(5)-C(88)	1.353(9)	N(5)-C(89)	1.383(9)
N(5)-C(91)	1.479(10)	N(6)-C(88)	1.371(8)
N(6)-C(90)	1.380(9)	N(6)-C(97)	1.469(9)
C(3)-C(4)	1.360(9)	C(5)-C(6)	1.529(9)
C(5)-C(10)	1.533(10)	C(6)-C(7)	1.513(9)
C(7)-C(8)	1.513(10)	C(8)-C(9)	1.542(10)
C(9)-C(10)	1.532(10)	C(11)-C(16)	1.478(10)
C(11)-C(12)	1.538(10)	C(12)-C(13)	1.530(11)
C(13)-C(14)	1.503(15)	C(14)-C(15)	1.505(14)
C(15)-C(16)	1.543(11)	C(17)-C(18)	1.523(11)
C(18)-C(19)	1.523(10)	C(20)-C(25)	1.332(14)
C(20)-C(21)	1.396(13)	C(21)-C(22)	1.389(14)
C(22)-C(23)	1.37(2)	C(23)-C(24)	1.43(2)
C(24)-C(25)	1.317(18)	C(26)-C(27)	1.351(11)
C(26)-C(31)	1.396(11)	C(27)-C(28)	1.396(11)
C(28)-C(29)	1.360(11)	C(29)-C(30)	1.359(13)
C(30)-C(31)	1.392(12)	C(32)-C(33)	1.385(10)
C(32)-C(37)	1.395(10)	C(33)-C(34)	1.382(10)
C(34)-C(35)	1.372(11)	C(35)-C(36)	1.364(11)
C(36)-C(37)	1.355(10)	C(38)-C(39)	1.384(11)
C(38)-C(43)	1.390(10)	C(39)-C(40)	1.379(10)
C(40)-C(41)	1.376(13)	C(41)-C(42)	1.354(13)
C(42)-C(43)	1.406(12)	C(46)-C(47)	1.339(10)
C(48)-C(49)	1.518(10)	C(48)-C(53)	1.527(10)
C(49)-C(50)	1.543(11)	C(50)-C(51)	1.538(12)
C(51)-C(52)	1.536(12)	C(52)-C(53)	1.549(10)
C(54)-C(59)	1.519(10)	C(54)-C(55)	1.521(10)
C(55)-C(56)	1.529(11)	C(56)-C(57)	1.490(12)
C(57)-C(58)	1.495(11)	C(58)-C(59)	1.508(11)
C(60)-C(61)	1.532(10)	C(61)-C(62)	1.544(10)
C(63)-C(64)	1.394(11)	C(63)-C(68)	1.401(12)
C(64)-C(65)	1.385(11)	C(65)-C(66)	1.419(14)
C(66)-C(67)	1.392(13)	C(67)-C(68)	1.391(11)
C(69)-C(70)	1.400(12)	C(69)-C(74)	1.433(12)
C(70)-C(71)	1.378(12)	C(71)-C(72)	1.315(17)
C(72)-C(73)	1.378(19)	C(73)-C(74)	1.445(17)
C(75)-C(80)	1.377(10)	C(75)-C(76)	1.410(10)
C(76)-C(77)	1.373(10)	C(77)-C(78)	1.365(11)
C(78)-C(79)	1.393(11)	C(79)-C(80)	1.385(10)
C(81)-C(86)	1.401(10)	C(81)-C(82)	1.403(10)
C(82)-C(83)	1.387(11)	C(83)-C(84)	1.379(11)
C(84)-C(85)	1.395(11)	C(85)-C(86)	1.357(10)
C(89)-C(90)	1.320(10)	C(91)-C(96)	1.492(11)
C(91)-C(92)	1.512(12)	C(92)-C(93)	1.487(14)
C(93)-C(94)	1.469(18)	C(94)-C(95)	1.598(18)
C(95)-C(96)	1.534(13)	C(97)-C(102)	1.517(10)
C(97)-C(98)	1.527(10)	C(98)-C(99)	1.506(11)
C(99)-C(100)	1.530(12)	C(100)-C(101)	1.505(11)
C(101)-C(102)	1.517(11)	C(103)-C(104)	1.524(9)
C(104)-C(105)	1.517(10)	C(106)-C(111)	1.373(10)
C(106)-C(107)	1.388(10)	C(107)-C(108)	1.385(10)
C(108)-C(109)	1.376(11)	C(109)-C(110)	1.356(12)

C(110)-C(111)	1.407(10)	C(112)-C(113)	1.422(10)
C(112)-C(117)	1.423(10)	C(113)-C(114)	1.383(10)
C(114)-C(115)	1.371(11)	C(115)-C(116)	1.391(11)
C(116)-C(117)	1.345(10)	C(118)-C(119)	1.376(12)
C(118)-C(123)	1.377(12)	C(119)-C(120)	1.386(13)
C(120)-C(121)	1.344(16)	C(121)-C(122)	1.377(16)
C(122)-C(123)	1.384(14)	C(124)-C(125)	1.371(11)
C(124)-C(129)	1.380(11)	C(125)-C(126)	1.438(13)
C(126)-C(127)	1.354(15)	C(127)-C(128)	1.339(14)
C(128)-C(129)	1.419(11)	C(201)-C(202)	1.494(10)
C(202)-C(203)	1.526(10)	C(203)-C(204)	1.491(9)
C(204)-C(205)	1.491(9)	C(205)-C(206)	1.496(10)
C(1)-Ru(1)-F(1)	175.9(3)	C(1)-Ru(1)-C(2)	90.7(3)
F(1)-Ru(1)-C(2)	89.2(2)	C(1)-Ru(1)-P(1)	96.5(2)
F(1)-Ru(1)-P(1)	82.79(12)	C(2)-Ru(1)-P(1)	165.27(19)
C(1)-Ru(1)-P(2)	101.1(2)	F(1)-Ru(1)-P(2)	82.95(11)
C(2)-Ru(1)-P(2)	99.16(18)	P(1)-Ru(1)-P(2)	92.11(7)
C(44)-Ru(2)-C(45)	92.4(3)	C(44)-Ru(2)-F(2)	174.3(3)
C(45)-Ru(2)-F(2)	89.1(2)	C(44)-Ru(2)-P(4)	95.4(2)
C(45)-Ru(2)-P(4)	167.47(19)	F(2)-Ru(2)-P(4)	82.26(11)
C(44)-Ru(2)-P(3)	103.3(2)	C(45)-Ru(2)-P(3)	96.51(18)
F(2)-Ru(2)-P(3)	81.94(11)	P(4)-Ru(2)-P(3)	91.32(7)
C(87)-Ru(3)-F(3)	174.4(3)	C(87)-Ru(3)-C(88)	92.9(3)
F(3)-Ru(3)-C(88)	89.2(2)	C(87)-Ru(3)-P(5)	95.9(2)
F(3)-Ru(3)-P(5)	81.10(11)	C(88)-Ru(3)-P(5)	166.1(2)
C(87)-Ru(3)-P(6)	102.4(2)	F(3)-Ru(3)-P(6)	82.43(11)
C(88)-Ru(3)-P(6)	97.11(19)	P(5)-Ru(3)-P(6)	91.52(7)
C(20)-P(1)-C(17)	107.4(5)	C(20)-P(1)-C(26)	101.8(4)
C(17)-P(1)-C(26)	95.8(4)	C(20)-P(1)-Ru(1)	116.1(3)
C(17)-P(1)-Ru(1)	116.8(3)	C(26)-P(1)-Ru(1)	116.3(3)
C(38)-P(2)-C(19)	101.4(4)	C(38)-P(2)-C(32)	103.3(3)
C(19)-P(2)-C(32)	99.5(3)	C(38)-P(2)-Ru(1)	122.7(2)
C(19)-P(2)-Ru(1)	109.7(3)	C(32)-P(2)-Ru(1)	116.8(2)
C(81)-P(3)-C(75)	107.2(3)	C(81)-P(3)-C(62)	99.2(3)
C(75)-P(3)-C(62)	99.5(3)	C(81)-P(3)-Ru(2)	115.8(2)
C(75)-P(3)-Ru(2)	121.1(2)	C(62)-P(3)-Ru(2)	110.6(3)
C(69)-P(4)-C(63)	100.6(4)	C(69)-P(4)-C(60)	98.7(4)
C(63)-P(4)-C(60)	104.1(4)	C(69)-P(4)-Ru(2)	115.8(3)
C(63)-P(4)-Ru(2)	117.5(2)	C(60)-P(4)-Ru(2)	117.1(3)
C(112)-P(5)-C(106)	99.9(3)	C(112)-P(5)-C(103)	98.2(3)
C(106)-P(5)-C(103)	105.1(3)	C(112)-P(5)-Ru(3)	115.9(2)
C(106)-P(5)-Ru(3)	118.9(2)	C(103)-P(5)-Ru(3)	115.7(2)
C(124)-P(6)-C(105)	99.1(3)	C(124)-P(6)-C(118)	106.3(4)
C(105)-P(6)-C(118)	100.4(3)	C(124)-P(6)-Ru(3)	115.9(2)
C(105)-P(6)-Ru(3)	110.1(2)	C(118)-P(6)-Ru(3)	121.7(3)
C(2)-N(1)-C(3)	110.9(5)	C(2)-N(1)-C(5)	128.2(6)
C(3)-N(1)-C(5)	120.9(5)	C(2)-N(2)-C(4)	111.1(5)
C(2)-N(2)-C(11)	126.5(6)	C(4)-N(2)-C(11)	122.1(6)
C(45)-N(3)-C(46)	111.1(6)	C(45)-N(3)-C(48)	125.7(6)
C(46)-N(3)-C(48)	123.2(6)	C(45)-N(4)-C(47)	112.3(6)
C(45)-N(4)-C(54)	124.9(6)	C(47)-N(4)-C(54)	122.6(6)
C(88)-N(5)-C(89)	111.0(6)	C(88)-N(5)-C(91)	126.4(6)
C(89)-N(5)-C(91)	122.5(7)	C(88)-N(6)-C(90)	110.9(6)
C(88)-N(6)-C(97)	125.6(6)	C(90)-N(6)-C(97)	123.3(6)

O(1)-C(1)-Ru(1)	177.8(7)	N(1)-C(2)-N(2)	104.8(5)
N(1)-C(2)-Ru(1)	132.3(5)	N(2)-C(2)-Ru(1)	122.8(5)
C(4)-C(3)-N(1)	107.3(6)	C(3)-C(4)-N(2)	105.9(6)
N(1)-C(5)-C(6)	110.8(6)	N(1)-C(5)-C(10)	111.3(6)
C(6)-C(5)-C(10)	111.0(6)	C(7)-C(6)-C(5)	110.4(6)
C(6)-C(7)-C(8)	112.0(6)	C(7)-C(8)-C(9)	110.0(6)
C(10)-C(9)-C(8)	111.3(6)	C(9)-C(10)-C(5)	110.2(6)
N(2)-C(11)-C(16)	111.6(6)	N(2)-C(11)-C(12)	108.6(6)
C(16)-C(11)-C(12)	113.2(6)	C(13)-C(12)-C(11)	111.5(7)
C(14)-C(13)-C(12)	110.5(9)	C(13)-C(14)-C(15)	113.2(8)
C(14)-C(15)-C(16)	111.0(7)	C(11)-C(16)-C(15)	108.6(7)
C(18)-C(17)-P(1)	117.3(6)	C(19)-C(18)-C(17)	114.2(7)
C(18)-C(19)-P(2)	113.4(5)	C(25)-C(20)-C(21)	117.2(10)
C(25)-C(20)-P(1)	126.2(10)	C(21)-C(20)-P(1)	116.6(7)
C(22)-C(21)-C(20)	121.7(12)	C(23)-C(22)-C(21)	118.7(15)
C(22)-C(23)-C(24)	118.1(13)	C(25)-C(24)-C(23)	120.1(15)
C(24)-C(25)-C(20)	124.0(15)	C(27)-C(26)-C(31)	118.5(8)
C(27)-C(26)-P(1)	121.9(6)	C(31)-C(26)-P(1)	119.5(7)
C(26)-C(27)-C(28)	120.9(8)	C(29)-C(28)-C(27)	120.5(9)
C(30)-C(29)-C(28)	119.7(9)	C(29)-C(30)-C(31)	120.3(9)
C(30)-C(31)-C(26)	120.2(9)	C(33)-C(32)-C(37)	118.6(7)
C(33)-C(32)-P(2)	125.1(6)	C(37)-C(32)-P(2)	116.2(5)
C(34)-C(33)-C(32)	119.6(7)	C(35)-C(34)-C(33)	120.7(8)
C(36)-C(35)-C(34)	119.4(8)	C(37)-C(36)-C(35)	121.0(8)
C(36)-C(37)-C(32)	120.5(7)	C(39)-C(38)-C(43)	116.6(7)
C(39)-C(38)-P(2)	120.7(5)	C(43)-C(38)-P(2)	122.6(6)
C(40)-C(39)-C(38)	122.1(8)	C(41)-C(40)-C(39)	120.2(9)
C(42)-C(41)-C(40)	119.5(9)	C(41)-C(42)-C(43)	120.3(9)
C(38)-C(43)-C(42)	121.1(9)	O(2)-C(44)-Ru(2)	177.5(6)
N(4)-C(45)-N(3)	102.6(6)	N(4)-C(45)-Ru(2)	125.7(5)
N(3)-C(45)-Ru(2)	131.7(5)	C(47)-C(46)-N(3)	107.3(6)
C(46)-C(47)-N(4)	106.8(6)	N(3)-C(48)-C(49)	112.0(6)
N(3)-C(48)-C(53)	111.7(6)	C(49)-C(48)-C(53)	110.1(6)
C(48)-C(49)-C(50)	109.2(6)	C(51)-C(50)-C(49)	110.0(7)
C(52)-C(51)-C(50)	109.6(7)	C(51)-C(52)-C(53)	111.6(7)
C(48)-C(53)-C(52)	109.3(6)	N(4)-C(54)-C(59)	111.3(6)
N(4)-C(54)-C(55)	110.6(6)	C(59)-C(54)-C(55)	111.0(6)
C(54)-C(55)-C(56)	111.3(7)	C(57)-C(56)-C(55)	110.9(8)
C(56)-C(57)-C(58)	111.6(7)	C(57)-C(58)-C(59)	111.7(7)
C(58)-C(59)-C(54)	108.8(7)	C(61)-C(60)-P(4)	116.7(5)
C(60)-C(61)-C(62)	113.4(6)	C(61)-C(62)-P(3)	112.0(5)
C(64)-C(63)-C(68)	119.3(7)	C(64)-C(63)-P(4)	117.0(6)
C(68)-C(63)-P(4)	123.7(6)	C(65)-C(64)-C(63)	120.4(8)
C(64)-C(65)-C(66)	120.0(8)	C(67)-C(66)-C(65)	119.6(8)
C(66)-C(67)-C(68)	119.7(9)	C(67)-C(68)-C(63)	120.9(9)
C(70)-C(69)-C(74)	116.3(9)	C(70)-C(69)-P(4)	122.4(6)
C(74)-C(69)-P(4)	121.1(8)	C(71)-C(70)-C(69)	124.8(9)
C(72)-C(71)-C(70)	119.1(12)	C(71)-C(72)-C(73)	121.1(12)
C(72)-C(73)-C(74)	122.0(12)	C(69)-C(74)-C(73)	116.5(12)
C(80)-C(75)-C(76)	117.7(7)	C(80)-C(75)-P(3)	118.7(5)
C(76)-C(75)-P(3)	122.8(6)	C(77)-C(76)-C(75)	120.9(8)
C(78)-C(77)-C(76)	120.4(7)	C(77)-C(78)-C(79)	120.1(7)
C(80)-C(79)-C(78)	119.3(7)	C(75)-C(80)-C(79)	121.6(7)
C(86)-C(81)-C(82)	117.8(7)	C(86)-C(81)-P(3)	115.7(5)
C(82)-C(81)-P(3)	126.5(6)	C(83)-C(82)-C(81)	120.8(7)

C(84)-C(83)-C(82)	119.8(7)	C(83)-C(84)-C(85)	119.8(8)
C(86)-C(85)-C(84)	120.4(8)	C(85)-C(86)-C(81)	121.3(7)
O(3)-C(87)-Ru(3)	175.9(7)	N(5)-C(88)-N(6)	103.5(6)
N(5)-C(88)-Ru(3)	132.9(5)	N(6)-C(88)-Ru(3)	123.6(5)
C(90)-C(89)-N(5)	107.6(7)	C(89)-C(90)-N(6)	107.0(7)
N(5)-C(91)-C(96)	112.2(7)	N(5)-C(91)-C(92)	111.7(7)
C(96)-C(91)-C(92)	111.0(7)	C(93)-C(92)-C(91)	110.0(9)
C(94)-C(93)-C(92)	112.2(12)	C(93)-C(94)-C(95)	110.2(10)
C(96)-C(95)-C(94)	109.0(10)	C(91)-C(96)-C(95)	110.3(9)
N(6)-C(97)-C(102)	111.7(6)	N(6)-C(97)-C(98)	110.6(6)
C(102)-C(97)-C(98)	110.9(6)	C(99)-C(98)-C(97)	111.9(7)
C(98)-C(99)-C(100)	110.7(8)	C(101)-C(100)-C(99)	111.3(7)
C(100)-C(101)-C(102)	111.0(7)	C(101)-C(102)-C(97)	109.4(7)
C(104)-C(103)-P(5)	116.3(5)	C(105)-C(104)-C(103)	112.7(6)
C(104)-C(105)-P(6)	113.9(5)	C(111)-C(106)-C(107)	120.1(6)
C(111)-C(106)-P(5)	122.9(5)	C(107)-C(106)-P(5)	117.0(5)
C(108)-C(107)-C(106)	120.5(7)	C(109)-C(108)-C(107)	119.7(8)
C(110)-C(109)-C(108)	119.5(7)	C(109)-C(110)-C(111)	121.9(8)
C(106)-C(111)-C(110)	118.1(7)	C(113)-C(112)-C(117)	116.3(7)
C(113)-C(112)-P(5)	120.7(5)	C(117)-C(112)-P(5)	123.0(6)
C(114)-C(113)-C(112)	120.9(7)	C(115)-C(114)-C(113)	120.1(8)
C(114)-C(115)-C(116)	120.4(7)	C(117)-C(116)-C(115)	120.4(8)
C(116)-C(117)-C(112)	121.9(8)	C(119)-C(118)-C(123)	118.6(8)
C(119)-C(118)-P(6)	119.3(7)	C(123)-C(118)-P(6)	121.6(7)
C(118)-C(119)-C(120)	120.0(10)	C(121)-C(120)-C(119)	122.7(12)
C(120)-C(121)-C(122)	116.6(10)	C(121)-C(122)-C(123)	122.8(10)
C(118)-C(123)-C(122)	119.2(10)	C(125)-C(124)-C(129)	116.8(8)
C(125)-C(124)-P(6)	127.4(7)	C(129)-C(124)-P(6)	115.8(6)
C(124)-C(125)-C(126)	120.9(9)	C(127)-C(126)-C(125)	119.9(10)
C(128)-C(127)-C(126)	120.6(10)	C(127)-C(128)-C(129)	119.7(10)
C(124)-C(129)-C(128)	122.1(8)	C(201)-C(202)-C(203)	104.9(9)
C(204)-C(203)-C(202)	104.7(8)	C(203)-C(204)-C(205)	105.7(8)
C(204)-C(205)-C(206)	107.5(9)		

Table 120. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(ICy)(dppp)(CO)HF **(79)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	40(1)	28(1)	26(1)	-1(1)	2(1)	15(1)
Ru(2)	34(1)	29(1)	25(1)	2(1)	0(1)	16(1)
Ru(3)	36(1)	27(1)	24(1)	2(1)	2(1)	13(1)
P(1)	59(1)	31(1)	31(1)	-2(1)	4(1)	16(1)
P(2)	45(1)	33(1)	29(1)	0(1)	3(1)	20(1)
P(3)	43(1)	33(1)	27(1)	3(1)	4(1)	20(1)
P(4)	42(1)	38(1)	35(1)	6(1)	-3(1)	18(1)
P(5)	38(1)	27(1)	24(1)	1(1)	1(1)	13(1)
P(6)	40(1)	39(1)	27(1)	6(1)	1(1)	19(1)
F(1)	43(2)	39(2)	31(2)	-5(2)	-1(2)	17(2)
F(2)	43(2)	34(2)	35(2)	4(2)	3(2)	24(2)
F(3)	39(2)	27(2)	27(2)	-2(2)	2(2)	14(2)
O(1)	57(4)	45(3)	64(4)	-4(3)	-15(3)	26(3)
O(2)	54(3)	34(3)	34(3)	4(2)	1(2)	24(3)
O(3)	71(4)	40(3)	55(4)	-4(3)	8(3)	30(3)

N(1)	24(3)	28(3)	29(3)	-6(3)	2(3)	8(3)
N(2)	37(4)	32(3)	26(3)	-1(3)	5(3)	14(3)
N(3)	38(4)	34(3)	35(4)	-2(3)	-2(3)	22(3)
N(4)	41(4)	32(3)	26(3)	-4(3)	-4(3)	19(3)
N(5)	43(4)	40(4)	43(4)	6(3)	15(3)	18(3)
N(6)	34(4)	24(3)	32(4)	4(3)	2(3)	6(3)
C(1)	52(5)	31(4)	35(4)	-4(3)	9(4)	16(4)
C(2)	36(4)	33(4)	26(4)	3(3)	0(3)	20(4)
C(3)	32(4)	30(4)	37(4)	-4(4)	1(4)	10(3)
C(4)	38(4)	33(4)	27(4)	-5(3)	-1(3)	14(4)
C(5)	30(4)	34(4)	33(4)	-3(3)	-1(3)	12(4)
C(6)	37(4)	33(4)	33(4)	9(3)	1(3)	15(4)
C(7)	45(5)	32(4)	55(5)	9(4)	13(4)	17(4)
C(8)	30(4)	44(5)	68(6)	14(4)	8(4)	14(4)
C(9)	34(5)	54(5)	52(5)	0(4)	-4(4)	16(4)
C(10)	38(4)	32(4)	45(5)	7(4)	2(4)	12(4)
C(11)	30(4)	27(4)	30(4)	-5(3)	2(3)	3(3)
C(12)	66(6)	53(5)	31(5)	4(4)	7(4)	14(5)
C(13)	77(8)	58(6)	43(5)	3(5)	10(5)	-17(6)
C(14)	44(6)	96(8)	43(6)	-16(6)	17(5)	-14(6)
C(15)	33(5)	77(7)	75(7)	-33(6)	1(5)	6(5)
C(16)	40(5)	67(6)	46(5)	-17(4)	-8(4)	24(4)
C(17)	74(6)	53(5)	35(5)	-16(4)	-3(4)	19(5)
C(18)	66(6)	55(5)	28(4)	-12(4)	-3(4)	24(5)
C(19)	66(6)	42(5)	29(4)	-1(4)	-3(4)	28(4)
C(20)	60(6)	32(5)	71(7)	-9(5)	11(5)	15(4)
C(21)	76(7)	67(6)	106(9)	-39(6)	-26(6)	49(6)
C(22)	99(9)	73(8)	188(15)	-50(9)	-52(10)	60(8)
C(23)	69(8)	55(8)	280(20)	-15(11)	19(12)	35(7)
C(24)	147(14)	95(10)	195(19)	55(11)	115(14)	73(10)
C(25)	115(10)	58(7)	164(13)	36(8)	81(10)	56(7)
C(26)	51(5)	28(4)	49(5)	-4(4)	-11(4)	12(4)
C(27)	47(5)	38(5)	52(5)	6(4)	-8(5)	16(4)
C(28)	51(6)	49(6)	76(7)	4(5)	-12(5)	20(5)
C(29)	55(6)	43(6)	87(7)	5(5)	-13(6)	12(5)
C(30)	64(7)	31(5)	93(8)	6(5)	9(6)	-6(5)
C(31)	75(7)	44(6)	69(6)	-6(5)	9(5)	20(5)
C(32)	53(5)	31(4)	27(4)	-2(3)	-3(4)	19(4)
C(33)	68(6)	39(5)	35(5)	9(4)	11(4)	31(4)
C(34)	83(7)	39(5)	43(5)	6(4)	12(5)	29(5)
C(35)	82(7)	47(5)	51(6)	-10(4)	-19(5)	41(5)
C(36)	50(5)	32(5)	52(5)	-5(4)	0(4)	23(4)
C(37)	52(5)	39(5)	35(5)	-6(4)	-9(4)	25(4)
C(38)	55(5)	24(4)	33(5)	10(3)	18(4)	14(4)
C(39)	42(5)	58(6)	50(5)	-4(4)	4(4)	22(4)
C(40)	44(5)	63(6)	65(6)	-6(5)	19(5)	18(4)
C(41)	44(6)	45(5)	90(8)	-18(5)	14(6)	10(5)
C(42)	75(7)	44(5)	76(7)	5(5)	35(6)	27(5)
C(43)	57(6)	42(5)	49(5)	7(4)	17(4)	19(4)
C(44)	40(5)	38(5)	30(4)	-10(4)	-3(3)	19(4)
C(45)	39(4)	28(4)	26(4)	4(3)	6(3)	18(3)
C(46)	30(4)	47(5)	37(4)	-10(4)	-12(4)	14(4)
C(47)	42(5)	39(4)	36(5)	-9(4)	-5(4)	17(4)
C(48)	40(5)	43(5)	34(4)	-2(4)	-4(3)	25(4)
C(49)	46(5)	44(5)	52(5)	-2(4)	2(4)	23(4)

C(50)	50(5)	79(6)	68(6)	-10(5)	3(5)	41(5)
C(51)	87(7)	76(7)	82(7)	0(6)	4(6)	66(6)
C(52)	75(7)	57(6)	73(6)	5(5)	7(5)	47(5)
C(53)	52(5)	55(5)	45(5)	4(4)	-1(4)	36(4)
C(54)	47(5)	41(4)	25(4)	-11(3)	-4(3)	29(4)
C(55)	75(6)	68(6)	41(5)	9(4)	7(4)	50(5)
C(56)	86(7)	102(8)	42(5)	0(5)	18(5)	68(7)
C(57)	103(8)	102(8)	41(5)	-3(5)	-1(5)	86(7)
C(58)	90(7)	72(6)	39(5)	-9(4)	-10(4)	64(6)
C(59)	73(6)	43(5)	38(5)	-8(4)	-8(4)	33(5)
C(60)	44(5)	45(5)	45(5)	8(4)	-14(4)	16(4)
C(61)	62(6)	38(5)	32(4)	4(4)	-8(4)	27(4)
C(62)	51(5)	43(5)	30(4)	9(4)	2(4)	22(4)
C(63)	36(5)	41(5)	56(6)	8(4)	-15(4)	11(4)
C(64)	63(5)	46(5)	42(5)	6(4)	-10(5)	22(4)
C(65)	79(7)	46(6)	63(6)	23(5)	-6(6)	10(5)
C(66)	83(7)	29(5)	89(8)	4(5)	-24(6)	13(5)
C(67)	100(8)	43(6)	64(6)	-1(5)	-17(6)	15(5)
C(68)	69(6)	44(5)	45(5)	4(5)	-5(5)	8(4)
C(69)	40(5)	54(5)	63(6)	33(5)	8(4)	21(4)
C(70)	58(6)	66(6)	54(6)	28(5)	14(5)	39(5)
C(71)	58(7)	102(8)	73(7)	44(6)	24(5)	59(7)
C(72)	108(12)	164(15)	106(11)	68(10)	52(9)	108(12)
C(73)	29(6)	151(13)	181(16)	84(12)	29(8)	47(8)
C(74)	45(6)	77(7)	111(9)	38(6)	-10(6)	20(6)
C(75)	50(5)	46(5)	25(4)	-2(3)	-1(3)	32(4)
C(76)	57(5)	55(5)	31(5)	-4(4)	4(4)	31(5)
C(77)	66(6)	66(6)	30(5)	-8(5)	2(4)	45(5)
C(78)	58(5)	52(6)	57(6)	-27(5)	-25(5)	38(5)
C(79)	78(6)	37(5)	34(5)	-11(4)	-5(4)	31(4)
C(80)	57(5)	43(5)	23(4)	7(4)	1(4)	31(4)
C(81)	41(4)	45(5)	29(4)	5(3)	7(3)	24(4)
C(82)	57(5)	50(5)	51(5)	2(4)	15(4)	33(5)
C(83)	48(5)	49(5)	69(6)	10(5)	16(5)	25(5)
C(84)	42(5)	36(5)	90(7)	8(5)	16(5)	11(4)
C(85)	49(5)	45(5)	67(6)	0(4)	-4(5)	24(5)
C(86)	41(5)	37(5)	39(5)	2(4)	4(4)	16(4)
C(87)	47(5)	36(5)	34(4)	4(4)	6(4)	20(4)
C(88)	38(4)	32(4)	21(4)	3(3)	-1(3)	14(4)
C(89)	41(5)	40(5)	42(5)	3(4)	14(4)	9(4)
C(90)	45(5)	39(4)	30(4)	2(3)	2(4)	17(4)
C(91)	55(6)	58(5)	56(5)	13(5)	16(4)	39(5)
C(92)	54(6)	102(8)	80(7)	20(6)	12(5)	46(6)
C(93)	99(10)	150(12)	124(12)	25(10)	7(8)	89(10)
C(94)	105(11)	182(16)	154(14)	69(13)	34(10)	110(12)
C(95)	172(14)	108(10)	116(10)	27(8)	37(9)	114(11)
C(96)	77(7)	68(6)	63(6)	7(5)	22(5)	42(5)
C(97)	41(4)	32(4)	32(4)	9(3)	5(3)	15(4)
C(98)	59(6)	63(6)	35(5)	-4(4)	-1(4)	29(5)
C(99)	71(6)	93(8)	36(5)	-4(5)	-18(5)	45(6)
C(100)	91(7)	85(7)	34(5)	12(5)	10(5)	55(6)
C(101)	84(7)	55(5)	35(5)	9(4)	5(4)	44(5)
C(102)	67(6)	39(5)	37(4)	3(4)	12(4)	28(4)
C(103)	36(4)	34(4)	29(4)	-6(3)	0(3)	16(4)
C(104)	42(5)	35(4)	26(4)	-3(3)	-6(3)	15(4)

C(105)	46(5)	38(4)	25(4)	-3(3)	-11(3)	19(4)
C(106)	37(4)	30(4)	27(4)	8(3)	8(3)	13(3)
C(107)	51(5)	35(4)	35(5)	10(4)	1(4)	16(4)
C(108)	99(7)	34(5)	43(6)	-15(4)	3(5)	22(5)
C(109)	99(7)	27(5)	56(6)	1(5)	15(5)	25(5)
C(110)	82(6)	42(5)	58(6)	17(5)	23(5)	34(5)
C(111)	56(5)	33(5)	39(5)	6(4)	6(4)	17(4)
C(112)	39(5)	22(4)	32(4)	-7(3)	-6(3)	11(4)
C(113)	50(5)	34(4)	33(5)	-6(4)	-3(4)	20(4)
C(114)	57(6)	47(5)	37(5)	-14(4)	-18(4)	32(5)
C(115)	46(5)	54(5)	57(6)	-27(5)	-29(5)	28(5)
C(116)	32(5)	43(5)	75(6)	-11(5)	-8(4)	14(4)
C(117)	39(5)	31(4)	58(5)	2(4)	0(4)	14(4)
C(118)	73(6)	74(6)	34(5)	20(4)	19(4)	55(5)
C(119)	124(9)	54(6)	51(6)	8(5)	2(6)	55(6)
C(120)	200(14)	77(8)	83(9)	18(7)	18(9)	98(9)
C(121)	210(16)	137(13)	55(8)	52(8)	41(9)	134(13)
C(122)	122(10)	148(12)	46(7)	25(7)	6(6)	97(10)
C(123)	107(8)	102(8)	37(5)	17(5)	7(5)	80(7)
C(124)	34(5)	59(6)	29(4)	8(4)	-4(3)	16(4)
C(125)	53(6)	85(7)	64(6)	17(6)	-4(5)	24(5)
C(126)	39(6)	120(10)	79(8)	2(8)	-12(5)	13(6)
C(127)	59(7)	83(8)	82(8)	17(6)	-3(6)	8(6)
C(128)	50(6)	54(6)	76(7)	11(5)	11(5)	6(5)
C(129)	37(5)	49(5)	42(5)	3(4)	3(4)	8(4)

Table 121. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(ICy)(dppp)(CO)HF **(79)**.

Atom	x	y	z	U(eq)
H(3D)	3931	-578	2168	42
H(4)	3237	-1013	2502	41
H(5)	4267	-973	352	41
H(6A)	4225	-417	101	43
H(6B)	4392	-261	1106	43
H(7A)	4888	36	22	54
H(7B)	4805	-373	-343	54
H(8A)	5099	-69	1437	59
H(8B)	5340	-119	629	59
H(9A)	4956	-794	712	59
H(9B)	5123	-636	1714	59
H(10A)	4535	-695	2174	49
H(10B)	4454	-1100	1785	49
H(11)	2857	-1893	1104	41
H(12A)	3088	-2023	2459	68
H(12B)	2952	-1779	3054	68
H(13A)	2457	-2497	2171	98
H(13B)	2489	-2420	3255	98
H(14A)	2203	-2048	3127	99
H(14B)	1933	-2446	2620	99
H(15A)	1995	-1929	1740	85
H(15B)	2158	-2160	1190	85
H(16A)	2602	-1492	1053	63
H(16B)	2629	-1448	2149	63

H(17A)	3148	-2616	-2128	72
H(17B)	2930	-2391	-1866	72
H(18A)	3715	-2014	-2404	63
H(18B)	3373	-2107	-3101	63
H(19A)	3223	-1710	-2077	54
H(19B)	3580	-1493	-2756	54
H(21)	3592	-2613	811	93
H(22)	3968	-2899	1014	135
H(23)	4288	-2961	-258	160
H(24)	4118	-2844	-1746	168
H(25)	3740	-2589	-1888	128
H(27)	2659	-2472	389	58
H(28)	2067	-2994	800	73
H(29)	1912	-3608	389	81
H(30)	2346	-3708	-423	91
H(31)	2934	-3187	-870	81
H(33)	4305	-632	-2011	55
H(34)	4278	-68	-1985	67
H(35)	3772	-51	-1272	67
H(36)	3298	-595	-559	52
H(37)	3311	-1157	-587	49
H(39)	4467	-1417	-513	61
H(40)	5048	-1312	-1076	73
H(41)	5225	-1110	-2583	78
H(42)	4804	-1049	-3539	79
H(43)	4205	-1174	-2990	62
H(46)	4991	1954	357	48
H(47)	4655	2307	740	49
H(48)	4434	1191	-1328	45
H(49A)	5198	1630	-633	57
H(49B)	5063	1717	-1595	57
H(50A)	4902	1090	-2136	74
H(50B)	5346	1328	-1864	74
H(51A)	5055	694	-1231	84
H(51B)	5213	1007	-426	84
H(52A)	4583	524	-46	75
H(52B)	4425	579	-1009	75
H(53A)	4274	900	146	56
H(53B)	4716	1143	446	56
H(54)	3718	1876	-448	42
H(55A)	3962	2057	1421	66
H(55B)	3638	1646	1060	66
H(56A)	3230	1885	698	81
H(56B)	3365	1999	1740	81
H(57A)	3813	2616	1311	80
H(57B)	3405	2520	909	80
H(58A)	3881	2821	-210	68
H(58B)	3571	2398	-534	68
H(59A)	4304	2604	229	59
H(59B)	4191	2507	-832	59
H(60A)	2870	924	-3704	57
H(60B)	3137	1359	-3401	57
H(61A)	3376	1170	-4696	52
H(61B)	3442	893	-4028	52
H(62A)	3818	1697	-3637	51

H(62B)	4007	1539	-4355	51
H(64)	2810	360	-928	63
H(65)	2475	-307	-937	86
H(66)	2370	-644	-2339	89
H(67)	2578	-302	-3721	93
H(68)	2891	367	-3703	75
H(70)	3067	1471	-962	67
H(71)	2603	1591	-411	83
H(72)	1990	1231	-893	130
H(73)	1813	717	-1862	143
H(74)	2282	585	-2517	99
H(76)	4373	1213	-4563	56
H(77)	4329	677	-5264	59
H(78)	3993	83	-4570	61
H(79)	3732	28	-3101	58
H(80)	3786	568	-2382	47
H(82)	4850	1565	-3555	60
H(83)	5426	2145	-3618	66
H(84)	5475	2689	-2923	71
H(85)	4942	2652	-2182	64
H(86)	4365	2091	-2186	49
H(89)	1643	-990	-4360	55
H(90)	2002	-1324	-4118	47
H(91)	2081	-265	-6194	62
H(92A)	1469	-815	-6332	91
H(92B)	1358	-735	-5332	91
H(93A)	1549	-233	-6857	135
H(93B)	1125	-493	-6461	135
H(94A)	1294	-148	-5112	156
H(94B)	1391	138	-5962	156
H(95A)	2064	331	-5873	135
H(95B)	1934	387	-4871	135
H(96A)	2288	52	-4786	80
H(96B)	1865	-204	-4377	80
H(97)	2896	-869	-5503	43
H(98A)	3022	-611	-4013	63
H(98B)	2736	-1023	-3585	63
H(99A)	3355	-910	-3404	78
H(99B)	3446	-810	-4471	78
H(10C)	3322	-1439	-4237	78
H(10D)	2924	-1556	-3743	78
H(10E)	2806	-1787	-5251	65
H(10F)	3083	-1365	-5640	65
H(10G)	2375	-1595	-4697	56
H(10H)	2438	-1515	-5779	56
H(10I)	3614	5	-8830	41
H(10J)	3343	-421	-8469	41
H(10K)	3042	51	-9063	44
H(10L)	3085	-237	-9740	44
H(10M)	2679	-741	-8625	45
H(10N)	2473	-590	-9306	45
H(107)	3696	631	-6074	51
H(108)	4051	1298	-6135	76
H(109)	4212	1607	-7552	76
H(110)	3992	1255	-8876	71

H(111)	3652	580	-8843	54
H(113)	3492	-486	-6045	47
H(114)	3992	-582	-5594	53
H(115)	4602	-197	-6177	61
H(116)	4721	290	-7222	63
H(117)	4241	395	-7673	53
H(119)	2694	383	-7327	86
H(120)	2663	887	-8007	129
H(121)	2392	827	-9429	136
H(122)	2088	223	-10110	110
H(123)	2093	-296	-9440	84
H(125)	1640	-633	-8306	86
H(126)	1056	-1228	-8204	110
H(127)	1055	-1760	-7635	104
H(128)	1616	-1726	-7195	82
H(129)	2191	-1131	-7205	59
H(20A)	6171	1307	-425	151
H(20B)	6320	1480	-1427	151
H(20E)	5871	1264	-1200	151
H(20F)	6416	1968	-363	295
H(6)	5959	1759	-217	295
H(7)	6329	2026	-1981	96
H(20G)	5873	1821	-1827	96
H(20C)	6419	2520	-947	125
H(20D)	5963	2315	-798	125
H(20J)	5877	2384	-2371	175
H(20K)	6329	2572	-2544	175
H(20H)	6169	3056	-2378	309
H(20I)	6444	3082	-1558	309
H(20L)	5994	2894	-1384	309
H(1)	3268(11)	-2078(10)	950(20)	6(13)
H(2)	3465(16)	1214(19)	-530(20)	50(20)
H(3)	3124(14)	-242(17)	-5630(30)	43(19)

Table 122. Dihedral angles [°] for Ru(ICy)(dppp)(CO)HF **(79)**.

Atom1 - Atom2 - Atom3 - Atom4	Dihedral
C(1) - Ru(1) - P(1) - C(20)	-4.7(4)
F(1) - Ru(1) - P(1) - C(20)	179.4(4)
C(2) - Ru(1) - P(1) - C(20)	-123.2(8)
P(2) - Ru(1) - P(1) - C(20)	96.8(4)
C(1) - Ru(1) - P(1) - C(17)	-133.0(4)
F(1) - Ru(1) - P(1) - C(17)	51.1(4)
C(2) - Ru(1) - P(1) - C(17)	108.5(8)
P(2) - Ru(1) - P(1) - C(17)	-31.6(3)
C(1) - Ru(1) - P(1) - C(26)	115.0(4)
F(1) - Ru(1) - P(1) - C(26)	-60.9(3)
C(2) - Ru(1) - P(1) - C(26)	-3.5(8)
P(2) - Ru(1) - P(1) - C(26)	-143.5(3)
C(1) - Ru(1) - P(2) - C(38)	16.8(4)
F(1) - Ru(1) - P(2) - C(38)	-162.7(3)
C(2) - Ru(1) - P(2) - C(38)	109.3(3)
P(1) - Ru(1) - P(2) - C(38)	-80.2(3)
C(1) - Ru(1) - P(2) - C(19)	135.5(4)

F(1) - Ru(1) - P(2) - C(19)	-44.0(3)
C(2) - Ru(1) - P(2) - C(19)	-132.0(3)
P(1) - Ru(1) - P(2) - C(19)	38.5(3)
C(1) - Ru(1) - P(2) - C(32)	-112.3(4)
F(1) - Ru(1) - P(2) - C(32)	68.2(3)
C(2) - Ru(1) - P(2) - C(32)	-19.8(3)
P(1) - Ru(1) - P(2) - C(32)	150.7(3)
C(44) - Ru(2) - P(3) - C(81)	-113.2(3)
C(45) - Ru(2) - P(3) - C(81)	-19.2(3)
F(2) - Ru(2) - P(3) - C(81)	69.0(3)
P(4) - Ru(2) - P(3) - C(81)	151.0(3)
C(44) - Ru(2) - P(3) - C(75)	19.3(4)
C(45) - Ru(2) - P(3) - C(75)	113.3(3)
F(2) - Ru(2) - P(3) - C(75)	-158.5(3)
P(4) - Ru(2) - P(3) - C(75)	-76.5(3)
C(44) - Ru(2) - P(3) - C(62)	135.0(4)
C(45) - Ru(2) - P(3) - C(62)	-131.0(3)
F(2) - Ru(2) - P(3) - C(62)	-42.8(3)
P(4) - Ru(2) - P(3) - C(62)	39.2(3)
C(44) - Ru(2) - P(4) - C(69)	108.4(4)
C(45) - Ru(2) - P(4) - C(69)	-19.4(9)
F(2) - Ru(2) - P(4) - C(69)	-66.4(3)
P(3) - Ru(2) - P(4) - C(69)	-148.1(3)
C(44) - Ru(2) - P(4) - C(63)	-10.5(4)
C(45) - Ru(2) - P(4) - C(63)	-138.3(9)
F(2) - Ru(2) - P(4) - C(63)	174.6(3)
P(3) - Ru(2) - P(4) - C(63)	93.0(3)
C(44) - Ru(2) - P(4) - C(60)	-135.7(4)
C(45) - Ru(2) - P(4) - C(60)	96.5(9)
F(2) - Ru(2) - P(4) - C(60)	49.5(3)
P(3) - Ru(2) - P(4) - C(60)	-32.2(3)
C(87) - Ru(3) - P(5) - C(112)	109.4(3)
F(3) - Ru(3) - P(5) - C(112)	-65.8(3)
C(88) - Ru(3) - P(5) - C(112)	-19.5(8)
P(6) - Ru(3) - P(5) - C(112)	-147.9(2)
C(87) - Ru(3) - P(5) - C(106)	-9.8(3)
F(3) - Ru(3) - P(5) - C(106)	175.0(3)
C(88) - Ru(3) - P(5) - C(106)	-138.7(8)
P(6) - Ru(3) - P(5) - C(106)	92.9(3)
C(87) - Ru(3) - P(5) - C(103)	-136.4(3)
F(3) - Ru(3) - P(5) - C(103)	48.3(3)
C(88) - Ru(3) - P(5) - C(103)	94.7(8)
P(6) - Ru(3) - P(5) - C(103)	-33.7(3)
C(87) - Ru(3) - P(6) - C(124)	-113.6(4)
F(3) - Ru(3) - P(6) - C(124)	69.2(3)
C(88) - Ru(3) - P(6) - C(124)	-19.1(4)
P(5) - Ru(3) - P(6) - C(124)	150.0(3)
C(87) - Ru(3) - P(6) - C(105)	135.0(3)
F(3) - Ru(3) - P(6) - C(105)	-42.2(3)
C(88) - Ru(3) - P(6) - C(105)	-130.5(3)
P(5) - Ru(3) - P(6) - C(105)	38.6(3)
C(87) - Ru(3) - P(6) - C(118)	18.2(4)
F(3) - Ru(3) - P(6) - C(118)	-159.1(3)
C(88) - Ru(3) - P(6) - C(118)	112.7(4)
P(5) - Ru(3) - P(6) - C(118)	-78.3(3)

F(1) - Ru(1) - C(1) - O(1)	-2(21)
C(2) - Ru(1) - C(1) - O(1)	86(18)
P(1) - Ru(1) - C(1) - O(1)	-81(18)
P(2) - Ru(1) - C(1) - O(1)	-174(100)
C(3) - N(1) - C(2) - N(2)	1.4(7)
C(5) - N(1) - C(2) - N(2)	178.8(6)
C(3) - N(1) - C(2) - Ru(1)	-177.8(5)
C(5) - N(1) - C(2) - Ru(1)	-0.4(10)
C(4) - N(2) - C(2) - N(1)	-0.4(7)
C(11) - N(2) - C(2) - N(1)	-174.7(6)
C(4) - N(2) - C(2) - Ru(1)	178.9(4)
C(11) - N(2) - C(2) - Ru(1)	4.6(9)
C(1) - Ru(1) - C(2) - N(1)	50.8(7)
F(1) - Ru(1) - C(2) - N(1)	-133.4(6)
P(1) - Ru(1) - C(2) - N(1)	169.9(4)
P(2) - Ru(1) - C(2) - N(1)	-50.6(6)
C(1) - Ru(1) - C(2) - N(2)	-128.3(6)
F(1) - Ru(1) - C(2) - N(2)	47.6(5)
P(1) - Ru(1) - C(2) - N(2)	-9.2(12)
P(2) - Ru(1) - C(2) - N(2)	130.3(5)
C(2) - N(1) - C(3) - C(4)	-1.9(8)
C(5) - N(1) - C(3) - C(4)	-179.5(6)
N(1) - C(3) - C(4) - N(2)	1.6(8)
C(2) - N(2) - C(4) - C(3)	-0.8(8)
C(11) - N(2) - C(4) - C(3)	173.9(6)
C(2) - N(1) - C(5) - C(6)	131.9(7)
C(3) - N(1) - C(5) - C(6)	-50.9(8)
C(2) - N(1) - C(5) - C(10)	-104.2(8)
C(3) - N(1) - C(5) - C(10)	73.0(8)
N(1) - C(5) - C(6) - C(7)	-179.1(6)
C(10) - C(5) - C(6) - C(7)	56.8(8)
C(5) - C(6) - C(7) - C(8)	-57.6(8)
C(6) - C(7) - C(8) - C(9)	56.8(8)
C(7) - C(8) - C(9) - C(10)	-55.9(9)
C(8) - C(9) - C(10) - C(5)	56.0(8)
N(1) - C(5) - C(10) - C(9)	179.9(6)
C(6) - C(5) - C(10) - C(9)	-56.3(8)
C(2) - N(2) - C(11) - C(16)	-138.3(7)
C(4) - N(2) - C(11) - C(16)	48.0(8)
C(2) - N(2) - C(11) - C(12)	96.3(8)
C(4) - N(2) - C(11) - C(12)	-77.5(8)
N(2) - C(11) - C(12) - C(13)	179.5(7)
C(16) - C(11) - C(12) - C(13)	55.0(9)
C(11) - C(12) - C(13) - C(14)	-50.6(10)
C(12) - C(13) - C(14) - C(15)	53.2(10)
C(13) - C(14) - C(15) - C(16)	-57.0(10)
N(2) - C(11) - C(16) - C(15)	-179.8(6)
C(12) - C(11) - C(16) - C(15)	-57.0(8)
C(14) - C(15) - C(16) - C(11)	57.4(9)
C(20) - P(1) - C(17) - C(18)	-85.3(7)
C(26) - P(1) - C(17) - C(18)	170.4(7)
Ru(1) - P(1) - C(17) - C(18)	47.2(8)
P(1) - C(17) - C(18) - C(19)	-68.2(9)
C(17) - C(18) - C(19) - P(2)	80.2(8)
C(38) - P(2) - C(19) - C(18)	65.4(6)

C(32) - P(2) - C(19) - C(18)	171.2(6)
Ru(1) - P(2) - C(19) - C(18)	-65.8(6)
C(17) - P(1) - C(20) - C(25)	12.2(10)
C(26) - P(1) - C(20) - C(25)	112.1(9)
Ru(1) - P(1) - C(20) - C(25)	-120.6(8)
C(17) - P(1) - C(20) - C(21)	-167.5(7)
C(26) - P(1) - C(20) - C(21)	-67.5(8)
Ru(1) - P(1) - C(20) - C(21)	59.7(7)
C(25) - C(20) - C(21) - C(22)	-0.3(15)
P(1) - C(20) - C(21) - C(22)	179.4(8)
C(20) - C(21) - C(22) - C(23)	3.8(17)
C(21) - C(22) - C(23) - C(24)	-6.0(19)
C(22) - C(23) - C(24) - C(25)	5(2)
C(23) - C(24) - C(25) - C(20)	-2(2)
C(21) - C(20) - C(25) - C(24)	-0.8(17)
P(1) - C(20) - C(25) - C(24)	179.5(10)
C(20) - P(1) - C(26) - C(27)	146.2(7)
C(17) - P(1) - C(26) - C(27)	-104.6(7)
Ru(1) - P(1) - C(26) - C(27)	19.1(8)
C(20) - P(1) - C(26) - C(31)	-35.3(8)
C(17) - P(1) - C(26) - C(31)	73.8(8)
Ru(1) - P(1) - C(26) - C(31)	-162.5(6)
C(31) - C(26) - C(27) - C(28)	-0.2(12)
P(1) - C(26) - C(27) - C(28)	178.3(6)
C(26) - C(27) - C(28) - C(29)	0.4(13)
C(27) - C(28) - C(29) - C(30)	0.2(14)
C(28) - C(29) - C(30) - C(31)	-1.0(16)
C(29) - C(30) - C(31) - C(26)	1.2(15)
C(27) - C(26) - C(31) - C(30)	-0.6(14)
P(1) - C(26) - C(31) - C(30)	-179.1(7)
C(38) - P(2) - C(32) - C(33)	7.9(7)
C(19) - P(2) - C(32) - C(33)	-96.2(7)
Ru(1) - P(2) - C(32) - C(33)	145.8(6)
C(38) - P(2) - C(32) - C(37)	-171.4(6)
C(19) - P(2) - C(32) - C(37)	84.4(6)
Ru(1) - P(2) - C(32) - C(37)	-33.5(6)
C(37) - C(32) - C(33) - C(34)	0.7(11)
P(2) - C(32) - C(33) - C(34)	-178.7(6)
C(32) - C(33) - C(34) - C(35)	-0.4(12)
C(33) - C(34) - C(35) - C(36)	0.4(12)
C(34) - C(35) - C(36) - C(37)	-0.9(12)
C(35) - C(36) - C(37) - C(32)	1.3(11)
C(33) - C(32) - C(37) - C(36)	-1.1(11)
P(2) - C(32) - C(37) - C(36)	178.3(6)
C(19) - P(2) - C(38) - C(39)	-140.7(6)
C(32) - P(2) - C(38) - C(39)	116.5(6)
Ru(1) - P(2) - C(38) - C(39)	-18.1(7)
C(19) - P(2) - C(38) - C(43)	37.5(7)
C(32) - P(2) - C(38) - C(43)	-65.2(7)
Ru(1) - P(2) - C(38) - C(43)	160.1(5)
C(43) - C(38) - C(39) - C(40)	-0.7(11)
P(2) - C(38) - C(39) - C(40)	177.6(6)
C(38) - C(39) - C(40) - C(41)	1.8(13)
C(39) - C(40) - C(41) - C(42)	-1.8(13)
C(40) - C(41) - C(42) - C(43)	0.6(13)

C(39) - C(38) - C(43) - C(42)	-0.5(11)
P(2) - C(38) - C(43) - C(42)	-178.7(6)
C(41) - C(42) - C(43) - C(38)	0.5(12)
C(45) - Ru(2) - C(44) - O(2)	123(14)
F(2) - Ru(2) - C(44) - O(2)	18(16)
P(4) - Ru(2) - C(44) - O(2)	-47(14)
P(3) - Ru(2) - C(44) - O(2)	-139(14)
C(47) - N(4) - C(45) - N(3)	0.0(7)
C(54) - N(4) - C(45) - N(3)	-175.3(6)
C(47) - N(4) - C(45) - Ru(2)	-179.1(5)
C(54) - N(4) - C(45) - Ru(2)	5.7(9)
C(46) - N(3) - C(45) - N(4)	0.1(7)
C(48) - N(3) - C(45) - N(4)	177.6(6)
C(46) - N(3) - C(45) - Ru(2)	179.0(5)
C(48) - N(3) - C(45) - Ru(2)	-3.5(10)
C(44) - Ru(2) - C(45) - N(4)	-132.0(6)
F(2) - Ru(2) - C(45) - N(4)	42.5(6)
P(4) - Ru(2) - C(45) - N(4)	-4.0(13)
P(3) - Ru(2) - C(45) - N(4)	124.3(5)
C(44) - Ru(2) - C(45) - N(3)	49.3(7)
F(2) - Ru(2) - C(45) - N(3)	-136.2(6)
P(4) - Ru(2) - C(45) - N(3)	177.3(5)
P(3) - Ru(2) - C(45) - N(3)	-54.4(6)
C(45) - N(3) - C(46) - C(47)	-0.1(8)
C(48) - N(3) - C(46) - C(47)	-177.7(6)
N(3) - C(46) - C(47) - N(4)	0.1(8)
C(45) - N(4) - C(47) - C(46)	0.0(8)
C(54) - N(4) - C(47) - C(46)	175.3(6)
C(45) - N(3) - C(48) - C(49)	135.9(7)
C(46) - N(3) - C(48) - C(49)	-46.9(9)
C(45) - N(3) - C(48) - C(53)	-100.0(8)
C(46) - N(3) - C(48) - C(53)	77.2(8)
N(3) - C(48) - C(49) - C(50)	-173.0(6)
C(53) - C(48) - C(49) - C(50)	62.0(8)
C(48) - C(49) - C(50) - C(51)	-60.9(9)
C(49) - C(50) - C(51) - C(52)	57.5(10)
C(50) - C(51) - C(52) - C(53)	-55.8(10)
N(3) - C(48) - C(53) - C(52)	175.4(6)
C(49) - C(48) - C(53) - C(52)	-59.5(8)
C(51) - C(52) - C(53) - C(48)	56.7(9)
C(45) - N(4) - C(54) - C(59)	-129.6(7)
C(47) - N(4) - C(54) - C(59)	55.6(8)
C(45) - N(4) - C(54) - C(55)	106.6(7)
C(47) - N(4) - C(54) - C(55)	-68.2(8)
N(4) - C(54) - C(55) - C(56)	179.5(7)
C(59) - C(54) - C(55) - C(56)	55.5(9)
C(54) - C(55) - C(56) - C(57)	-53.6(10)
C(55) - C(56) - C(57) - C(58)	54.7(10)
C(56) - C(57) - C(58) - C(59)	-58.4(11)
C(57) - C(58) - C(59) - C(54)	58.7(9)
N(4) - C(54) - C(59) - C(58)	179.2(6)
C(55) - C(54) - C(59) - C(58)	-57.2(8)
C(69) - P(4) - C(60) - C(61)	173.8(6)
C(63) - P(4) - C(60) - C(61)	-82.9(6)
Ru(2) - P(4) - C(60) - C(61)	48.8(6)

P(4) - C(60) - C(61) - C(62)	-70.0(7)
C(60) - C(61) - C(62) - P(3)	80.9(7)
C(81) - P(3) - C(62) - C(61)	171.5(5)
C(75) - P(3) - C(62) - C(61)	62.2(6)
Ru(2) - P(3) - C(62) - C(61)	-66.3(6)
C(69) - P(4) - C(63) - C(64)	-63.8(7)
C(60) - P(4) - C(63) - C(64)	-165.7(6)
Ru(2) - P(4) - C(63) - C(64)	62.9(7)
C(69) - P(4) - C(63) - C(68)	116.4(7)
C(60) - P(4) - C(63) - C(68)	14.5(8)
Ru(2) - P(4) - C(63) - C(68)	-116.9(7)
C(68) - C(63) - C(64) - C(65)	-1.6(12)
P(4) - C(63) - C(64) - C(65)	178.6(7)
C(63) - C(64) - C(65) - C(66)	2.3(14)
C(64) - C(65) - C(66) - C(67)	-1.6(15)
C(65) - C(66) - C(67) - C(68)	0.2(15)
C(66) - C(67) - C(68) - C(63)	0.5(15)
C(64) - C(63) - C(68) - C(67)	0.2(13)
P(4) - C(63) - C(68) - C(67)	-180.0(7)
C(63) - P(4) - C(69) - C(70)	145.5(6)
C(60) - P(4) - C(69) - C(70)	-108.2(7)
Ru(2) - P(4) - C(69) - C(70)	17.7(7)
C(63) - P(4) - C(69) - C(74)	-39.8(7)
C(60) - P(4) - C(69) - C(74)	66.4(7)
Ru(2) - P(4) - C(69) - C(74)	-167.7(6)
C(74) - C(69) - C(70) - C(71)	1.3(12)
P(4) - C(69) - C(70) - C(71)	176.2(6)
C(69) - C(70) - C(71) - C(72)	-0.8(14)
C(70) - C(71) - C(72) - C(73)	1.6(17)
C(71) - C(72) - C(73) - C(74)	-3(2)
C(70) - C(69) - C(74) - C(73)	-2.4(12)
P(4) - C(69) - C(74) - C(73)	-177.4(7)
C(72) - C(73) - C(74) - C(69)	3.4(17)
C(81) - P(3) - C(75) - C(80)	137.1(6)
C(62) - P(3) - C(75) - C(80)	-120.1(6)
Ru(2) - P(3) - C(75) - C(80)	1.0(7)
C(81) - P(3) - C(75) - C(76)	-53.2(7)
C(62) - P(3) - C(75) - C(76)	49.6(7)
Ru(2) - P(3) - C(75) - C(76)	170.8(5)
C(80) - C(75) - C(76) - C(77)	-1.3(11)
P(3) - C(75) - C(76) - C(77)	-171.2(6)
C(75) - C(76) - C(77) - C(78)	2.0(12)
C(76) - C(77) - C(78) - C(79)	-2.1(12)
C(77) - C(78) - C(79) - C(80)	1.4(12)
C(76) - C(75) - C(80) - C(79)	0.7(11)
P(3) - C(75) - C(80) - C(79)	171.0(6)
C(78) - C(79) - C(80) - C(75)	-0.7(11)
C(75) - P(3) - C(81) - C(86)	-177.4(5)
C(62) - P(3) - C(81) - C(86)	79.5(6)
Ru(2) - P(3) - C(81) - C(86)	-38.8(6)
C(75) - P(3) - C(81) - C(82)	4.0(7)
C(62) - P(3) - C(81) - C(82)	-99.1(7)
Ru(2) - P(3) - C(81) - C(82)	142.7(6)
C(86) - C(81) - C(82) - C(83)	-2.5(11)
P(3) - C(81) - C(82) - C(83)	176.1(6)

C(81) - C(82) - C(83) - C(84)	2.3(13)
C(82) - C(83) - C(84) - C(85)	-0.3(13)
C(83) - C(84) - C(85) - C(86)	-1.5(13)
C(84) - C(85) - C(86) - C(81)	1.3(12)
C(82) - C(81) - C(86) - C(85)	0.6(11)
P(3) - C(81) - C(86) - C(85)	-178.1(6)
F(3) - Ru(3) - C(87) - O(3)	-36(12)
C(88) - Ru(3) - C(87) - O(3)	76(10)
P(5) - Ru(3) - C(87) - O(3)	-93(10)
P(6) - Ru(3) - C(87) - O(3)	174(100)
C(89) - N(5) - C(88) - N(6)	1.3(8)
C(91) - N(5) - C(88) - N(6)	177.9(7)
C(89) - N(5) - C(88) - Ru(3)	-177.7(5)
C(91) - N(5) - C(88) - Ru(3)	-1.1(11)
C(90) - N(6) - C(88) - N(5)	0.3(7)
C(97) - N(6) - C(88) - N(5)	-174.6(6)
C(90) - N(6) - C(88) - Ru(3)	179.4(5)
C(97) - N(6) - C(88) - Ru(3)	4.6(9)
C(87) - Ru(3) - C(88) - N(5)	48.0(7)
F(3) - Ru(3) - C(88) - N(5)	-137.2(7)
P(5) - Ru(3) - C(88) - N(5)	177.2(5)
P(6) - Ru(3) - C(88) - N(5)	-54.9(7)
C(87) - Ru(3) - C(88) - N(6)	-130.9(6)
F(3) - Ru(3) - C(88) - N(6)	43.9(5)
P(5) - Ru(3) - C(88) - N(6)	-1.7(12)
P(6) - Ru(3) - C(88) - N(6)	126.2(5)
C(88) - N(5) - C(89) - C(90)	-2.5(9)
C(91) - N(5) - C(89) - C(90)	-179.3(7)
N(5) - C(89) - C(90) - N(6)	2.6(8)
C(88) - N(6) - C(90) - C(89)	-1.8(8)
C(97) - N(6) - C(90) - C(89)	173.2(6)
C(88) - N(5) - C(91) - C(96)	-99.8(9)
C(89) - N(5) - C(91) - C(96)	76.4(9)
C(88) - N(5) - C(91) - C(92)	134.8(8)
C(89) - N(5) - C(91) - C(92)	-48.9(10)
N(5) - C(91) - C(92) - C(93)	-174.2(9)
C(96) - C(91) - C(92) - C(93)	59.7(11)
C(91) - C(92) - C(93) - C(94)	-59.3(13)
C(92) - C(93) - C(94) - C(95)	56.9(15)
C(93) - C(94) - C(95) - C(96)	-54.4(14)
N(5) - C(91) - C(96) - C(95)	175.0(8)
C(92) - C(91) - C(96) - C(95)	-59.2(11)
C(94) - C(95) - C(96) - C(91)	55.5(12)
C(88) - N(6) - C(97) - C(102)	-130.0(7)
C(90) - N(6) - C(97) - C(102)	55.7(8)
C(88) - N(6) - C(97) - C(98)	106.0(7)
C(90) - N(6) - C(97) - C(98)	-68.2(8)
N(6) - C(97) - C(98) - C(99)	-179.6(7)
C(102) - C(97) - C(98) - C(99)	55.9(9)
C(97) - C(98) - C(99) - C(100)	-53.6(9)
C(98) - C(99) - C(100) - C(101)	54.5(10)
C(99) - C(100) - C(101) - C(102)	-57.7(10)
C(100) - C(101) - C(102) - C(97)	58.9(9)
N(6) - C(97) - C(102) - C(101)	178.7(6)
C(98) - C(97) - C(102) - C(101)	-57.5(8)

C(112) - P(5) - C(103) - C(104)	175.9(5)
C(106) - P(5) - C(103) - C(104)	-81.5(6)
Ru(3) - P(5) - C(103) - C(104)	51.8(6)
P(5) - C(103) - C(104) - C(105)	-71.6(7)
C(103) - C(104) - C(105) - P(6)	80.9(7)
C(124) - P(6) - C(105) - C(104)	172.6(5)
C(118) - P(6) - C(105) - C(104)	64.1(6)
Ru(3) - P(6) - C(105) - C(104)	-65.4(5)
C(112) - P(5) - C(106) - C(111)	108.6(7)
C(103) - P(5) - C(106) - C(111)	7.3(7)
Ru(3) - P(5) - C(106) - C(111)	-124.2(6)
C(112) - P(5) - C(106) - C(107)	-70.0(6)
C(103) - P(5) - C(106) - C(107)	-171.3(6)
Ru(3) - P(5) - C(106) - C(107)	57.1(6)
C(111) - C(106) - C(107) - C(108)	-2.8(12)
P(5) - C(106) - C(107) - C(108)	175.8(6)
C(106) - C(107) - C(108) - C(109)	1.1(13)
C(107) - C(108) - C(109) - C(110)	1.8(15)
C(108) - C(109) - C(110) - C(111)	-3.1(14)
C(107) - C(106) - C(111) - C(110)	1.6(11)
P(5) - C(106) - C(111) - C(110)	-177.0(6)
C(109) - C(110) - C(111) - C(106)	1.4(13)
C(106) - P(5) - C(112) - C(113)	145.1(5)
C(103) - P(5) - C(112) - C(113)	-107.9(6)
Ru(3) - P(5) - C(112) - C(113)	16.0(6)
C(106) - P(5) - C(112) - C(117)	-36.8(6)
C(103) - P(5) - C(112) - C(117)	70.2(6)
Ru(3) - P(5) - C(112) - C(117)	-165.9(5)
C(117) - C(112) - C(113) - C(114)	-1.3(10)
P(5) - C(112) - C(113) - C(114)	176.9(5)
C(112) - C(113) - C(114) - C(115)	0.5(10)
C(113) - C(114) - C(115) - C(116)	0.2(11)
C(114) - C(115) - C(116) - C(117)	0.1(12)
C(115) - C(116) - C(117) - C(112)	-1.0(12)
C(113) - C(112) - C(117) - C(116)	1.6(11)
P(5) - C(112) - C(117) - C(116)	-176.7(6)
C(124) - P(6) - C(118) - C(119)	134.2(7)
C(105) - P(6) - C(118) - C(119)	-123.0(7)
Ru(3) - P(6) - C(118) - C(119)	-1.4(8)
C(124) - P(6) - C(118) - C(123)	-53.9(8)
C(105) - P(6) - C(118) - C(123)	48.8(8)
Ru(3) - P(6) - C(118) - C(123)	170.4(6)
C(123) - C(118) - C(119) - C(120)	1.6(14)
P(6) - C(118) - C(119) - C(120)	173.6(8)
C(118) - C(119) - C(120) - C(121)	-3.0(18)
C(119) - C(120) - C(121) - C(122)	3(2)
C(120) - C(121) - C(122) - C(123)	-2.0(19)
C(119) - C(118) - C(123) - C(122)	-0.5(13)
P(6) - C(118) - C(123) - C(122)	-172.4(7)
C(121) - C(122) - C(123) - C(118)	0.8(16)
C(105) - P(6) - C(124) - C(125)	-104.0(8)
C(118) - P(6) - C(124) - C(125)	-0.4(9)
Ru(3) - P(6) - C(124) - C(125)	138.3(7)
C(105) - P(6) - C(124) - C(129)	75.3(6)
C(118) - P(6) - C(124) - C(129)	179.0(6)

Ru(3) - P(6) - C(124) - C(129)	-42.3(7)
C(129) - C(124) - C(125) - C(126)	-0.1(13)
P(6) - C(124) - C(125) - C(126)	179.3(7)
C(124) - C(125) - C(126) - C(127)	-0.8(16)
C(125) - C(126) - C(127) - C(128)	-0.5(18)
C(126) - C(127) - C(128) - C(129)	2.6(17)
C(125) - C(124) - C(129) - C(128)	2.2(12)
P(6) - C(124) - C(129) - C(128)	-177.3(7)
C(127) - C(128) - C(129) - C(124)	-3.5(14)
C(201) - C(202) - C(203) - C(204)	-179.2(19)
C(202) - C(203) - C(204) - C(205)	180(2)
C(203) - C(204) - C(205) - C(206)	-177.6(19)

Table 123. Crystal data and structure refinement for Ru(ICy)(dppp)(CO)(C_6F_5)H **(80)**.

Compound	Ru(ICy)(dppp)(CO)(C_6F_5)H **(80)**
Empirical formula	C49 H51 F5 N2 O P2 Ru
Formula weight	941.93
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 12.4090(3)Å α = 83.783(1)^o
	b = 13.8650(3)Å β = 66.562(1)^o
	c = 13.9590(3)Å γ = 88.922(1)^o
Volume	2189.77(9) Å^3
Z	2
Density (calculated)	1.429 Mg/m^3
Absorption coefficient	0.492 mm^{-1}
F(000)	972
Crystal size	0.25 x 0.20 x 0.15 mm
Theta range for data collection	3.51 to 27.48^o
Index ranges	-16<=h<=16; -18<=k<=18; -18<=l<=18
Reflections collected	36187
Independent reflections	9954 [R(int) = 0.0759]
Reflections observed (>2σ)	6800
Data Completeness	0.994
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.95 and 0.83
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9954 / 1 / 545
Goodness-of-fit on F^2	1.019
Final R indices [I>2σ(I)]	R1 = 0.0436 wR2 = 0.0818
R indices (all data)	R1 = 0.0860 wR2 = 0.0958
Largest diff. peak and hole	1.021 and -1.179 eÅ^{-3}

Table 124. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ru(ICy)(dppp)(CO)(C_6F_5)H **(80)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	X	y	z	U(eq)
Ru(1)	2600(1)	2711(1)	2506(1)	18(1)
P(1)	3177(1)	3845(1)	3322(1)	19(1)
P(2)	839(1)	3445(1)	2743(1)	19(1)
F(1)	1185(2)	535(1)	3297(2)	47(1)
F(2)	640(2)	-778(1)	2330(2)	71(1)
F(3)	1232(2)	-507(2)	218(2)	94(1)
F(4)	2411(2)	1158(2)	-906(2)	75(1)
F(5)	2977(2)	2503(1)	14(1)	41(1)
O(1)	3774(2)	4223(1)	612(2)	32(1)
N(1)	4031(2)	1146(2)	3335(2)	26(1)
N(2)	4929(2)	1523(2)	1669(2)	26(1)
C(1)	3379(2)	3588(2)	1268(2)	22(1)
C(2)	3962(2)	1755(2)	2510(2)	20(1)
C(3)	5008(3)	577(2)	2995(2)	41(1)
C(4)	5571(3)	817(2)	1963(3)	44(1)
C(5)	3193(2)	1016(2)	4447(2)	28(1)
C(6)	2638(3)	8(3)	4716(3)	53(1)
C(7)	1727(4)	-140(4)	5843(3)	79(2)
C(8)	2288(3)	17(3)	6611(3)	51(1)
C(9)	2885(3)	1007(3)	6339(3)	49(1)
C(10)	3765(3)	1185(2)	5198(2)	38(1)
C(11)	5334(2)	2001(2)	583(2)	24(1)
C(12)	6376(3)	2675(2)	361(2)	32(1)
C(13)	6800(3)	3188(2)	-745(2)	34(1)
C(14)	7103(3)	2468(2)	-1554(2)	41(1)
C(15)	6048(3)	1801(2)	-1326(2)	44(1)
C(16)	5617(3)	1272(2)	-218(2)	35(1)
C(17)	2129(2)	1618(2)	1726(2)	22(1)
C(18)	2395(3)	1697(2)	658(3)	34(1)
C(19)	2103(3)	1005(3)	142(3)	49(1)
C(20)	1508(3)	175(3)	712(4)	59(1)
C(21)	1222(3)	51(2)	1757(4)	50(1)
C(22)	1541(3)	749(2)	2233(3)	38(1)
C(23)	4778(2)	4058(2)	2775(2)	21(1)
C(24)	5473(2)	3371(2)	3047(2)	25(1)
C(25)	6685(2)	3455(2)	2606(2)	26(1)
C(26)	7234(2)	4238(2)	1869(2)	28(1)
C(27)	6569(3)	4924(2)	1583(2)	27(1)
C(28)	5348(2)	4840(2)	2029(2)	25(1)
C(29)	2811(2)	3733(2)	4740(2)	23(1)
C(30)	1730(3)	3318(2)	5430(2)	28(1)
C(31)	1390(3)	3283(2)	6519(2)	37(1)
C(32)	2135(3)	3652(2)	6911(3)	42(1)
C(33)	3206(3)	4071(2)	6238(2)	40(1)
C(34)	3536(3)	4123(2)	5164(2)	32(1)
C(35)	2638(2)	5070(2)	3153(2)	22(1)
C(36)	1302(2)	5114(2)	3521(2)	24(1)
C(37)	849(2)	4773(2)	2741(2)	23(1)
C(38)	-504(2)	3098(2)	3927(2)	20(1)

C(39)	-1554(2)	3554(2)	4041(2)	26(1)
C(40)	-2588(3)	3290(2)	4895(2)	30(1)
C(41)	-2591(3)	2574(2)	5669(2)	34(1)
C(42)	-1561(3)	2126(2)	5580(2)	36(1)
C(43)	-523(3)	2371(2)	4700(2)	29(1)
C(44)	314(2)	3279(2)	1715(2)	20(1)
C(45)	671(2)	3895(2)	779(2)	25(1)
C(46)	364(3)	3685(2)	-30(2)	31(1)
C(47)	-293(3)	2864(2)	65(2)	32(1)
C(48)	-660(3)	2246(2)	997(2)	30(1)
C(49)	-367(2)	2449(2)	1807(2)	24(1)

Table 125. Bond lengths [Å] and angles [°] for Ru(ICy)(dppp)(CO)(C_6F_5)H **(80)**.

Ru(1)-C(1)	1.913(3)	Ru(1)-C(2)	2.130(3)
Ru(1)-C(17)	2.172(3)	Ru(1)-P(2)	2.3103(8)
Ru(1)-P(1)	2.3160(8)	Ru(1)-H(1)	1.600(5)
P(1)-C(29)	1.835(3)	P(1)-C(23)	1.839(3)
P(1)-C(35)	1.840(3)	P(2)-C(44)	1.832(3)
P(2)-C(37)	1.841(3)	P(2)-C(38)	1.845(3)
F(1)-C(22)	1.369(4)	F(2)-C(21)	1.362(4)
F(3)-C(20)	1.353(4)	F(4)-C(19)	1.350(4)
F(5)-C(18)	1.368(4)	O(1)-C(1)	1.157(3)
N(1)-C(3)	1.380(4)	N(1)-C(2)	1.383(3)
N(1)-C(5)	1.478(3)	N(2)-C(2)	1.367(3)
N(2)-C(4)	1.380(4)	N(2)-C(11)	1.477(3)
C(3)-C(4)	1.334(4)	C(3)-H(3)	0.9500
C(4)-H(4)	0.9500	C(5)-C(6)	1.512(4)
C(5)-C(10)	1.519(4)	C(5)-H(5)	1.0000
C(6)-C(7)	1.523(5)	C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900	C(7)-C(8)	1.527(5)
C(7)-H(7A)	0.9900	C(7)-H(7B)	0.9900
C(8)-C(9)	1.509(5)	C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900	C(9)-C(10)	1.527(4)
C(9)-H(9A)	0.9900	C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900	C(10)-H(10B)	0.9900
C(11)-C(12)	1.519(4)	C(11)-C(16)	1.521(4)
C(11)-H(11)	1.0000	C(12)-C(13)	1.516(4)
C(12)-H(12A)	0.9900	C(12)-H(12B)	0.9900
C(13)-C(14)	1.518(4)	C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900	C(14)-C(15)	1.523(5)
C(14)-H(14A)	0.9900	C(14)-H(14B)	0.9900
C(15)-C(16)	1.526(4)	C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900	C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900	C(17)-C(18)	1.386(4)
C(17)-C(22)	1.386(4)	C(18)-C(19)	1.393(4)
C(19)-C(20)	1.367(6)	C(20)-C(21)	1.348(6)
C(21)-C(22)	1.377(5)	C(23)-C(24)	1.395(4)
C(23)-C(28)	1.400(4)	C(24)-C(25)	1.382(4)
C(24)-H(24)	0.9500	C(25)-C(26)	1.389(4)
C(25)-H(25)	0.9500	C(26)-C(27)	1.376(4)
C(26)-H(26)	0.9500	C(27)-C(28)	1.392(4)
C(27)-H(27)	0.9500	C(28)-H(28)	0.9500
C(29)-C(30)	1.393(4)	C(29)-C(34)	1.401(4)
C(30)-C(31)	1.401(4)	C(30)-H(30)	0.9500

C(31)-C(32)	1.377(5)	C(31)-H(31)	0.9500
C(32)-C(33)	1.379(5)	C(32)-H(32)	0.9500
C(33)-C(34)	1.382(4)	C(33)-H(33)	0.9500
C(34)-H(34)	0.9500	C(35)-C(36)	1.530(4)
C(35)-H(35A)	0.9900	C(35)-H(35B)	0.9900
C(36)-C(37)	1.528(4)	C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900	C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900	C(38)-C(43)	1.389(4)
C(38)-C(39)	1.396(4)	C(39)-C(40)	1.381(4)
C(39)-H(39)	0.9500	C(40)-C(41)	1.385(4)
C(40)-H(40)	0.9500	C(41)-C(42)	1.376(4)
C(41)-H(41)	0.9500	C(42)-C(43)	1.397(4)
C(42)-H(42)	0.9500	C(43)-H(43)	0.9500
C(44)-C(45)	1.395(4)	C(44)-C(49)	1.404(4)
C(45)-C(46)	1.388(4)	C(45)-H(45)	0.9500
C(46)-C(47)	1.377(4)	C(46)-H(46)	0.9500
C(47)-C(48)	1.390(4)	C(47)-H(47)	0.9500
C(48)-C(49)	1.375(4)	C(48)-H(48)	0.9500
C(49)-H(49)	0.9500		
C(1)-Ru(1)-C(2)	102.50(11)	C(1)-Ru(1)-C(17)	96.15(11)
C(2)-Ru(1)-C(17)	84.99(10)	C(1)-Ru(1)-P(2)	89.95(8)
C(2)-Ru(1)-P(2)	166.54(7)	C(17)-Ru(1)-P(2)	88.65(7)
C(1)-Ru(1)-P(1)	83.75(8)	C(2)-Ru(1)-P(1)	92.67(7)
C(17)-Ru(1)-P(1)	177.57(7)	P(2)-Ru(1)-P(1)	93.77(3)
C(1)-Ru(1)-H(1)	173.7(9)	C(2)-Ru(1)-H(1)	83.0(9)
C(17)-Ru(1)-H(1)	87.3(9)	P(2)-Ru(1)-H(1)	84.9(9)
P(1)-Ru(1)-H(1)	93.0(9)	C(29)-P(1)-C(23)	101.79(13)
C(29)-P(1)-C(35)	99.47(13)	C(23)-P(1)-C(35)	102.26(13)
C(29)-P(1)-Ru(1)	123.53(9)	C(23)-P(1)-Ru(1)	113.07(9)
C(35)-P(1)-Ru(1)	113.86(9)	C(44)-P(2)-C(37)	102.76(13)
C(44)-P(2)-C(38)	100.33(12)	C(37)-P(2)-C(38)	100.70(13)
C(44)-P(2)-Ru(1)	113.75(9)	C(37)-P(2)-Ru(1)	115.64(9)
C(38)-P(2)-Ru(1)	120.98(9)	C(3)-N(1)-C(2)	111.1(2)
C(3)-N(1)-C(5)	120.1(2)	C(2)-N(1)-C(5)	128.8(2)
C(2)-N(2)-C(4)	111.7(2)	C(2)-N(2)-C(11)	126.2(2)
C(4)-N(2)-C(11)	122.0(2)	O(1)-C(1)-Ru(1)	170.0(2)
N(2)-C(2)-N(1)	102.9(2)	N(2)-C(2)-Ru(1)	127.97(19)
N(1)-C(2)-Ru(1)	128.89(19)	C(4)-C(3)-N(1)	107.2(3)
C(4)-C(3)-H(3)	126.4	N(1)-C(3)-H(3)	126.4
C(3)-C(4)-N(2)	107.1(3)	C(3)-C(4)-H(4)	126.4
N(2)-C(4)-H(4)	126.4	N(1)-C(5)-C(6)	109.8(3)
N(1)-C(5)-C(10)	112.6(2)	C(6)-C(5)-C(10)	109.7(2)
N(1)-C(5)-H(5)	108.2	C(6)-C(5)-H(5)	108.2
C(10)-C(5)-H(5)	108.2	C(5)-C(6)-C(7)	111.4(3)
C(5)-C(6)-H(6A)	109.3	C(7)-C(6)-H(6A)	109.3
C(5)-C(6)-H(6B)	109.3	C(7)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	108.0	C(6)-C(7)-C(8)	110.5(3)
C(6)-C(7)-H(7A)	109.5	C(8)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5	C(8)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1	C(9)-C(8)-C(7)	110.0(3)
C(9)-C(8)-H(8A)	109.7	C(7)-C(8)-H(8A)	109.7
C(9)-C(8)-H(8B)	109.7	C(7)-C(8)-H(8B)	109.7
H(8A)-C(8)-H(8B)	108.2	C(8)-C(9)-C(10)	113.1(3)
C(8)-C(9)-H(9A)	109.0	C(10)-C(9)-H(9A)	109.0

C(8)-C(9)-H(9B)	109.0	C(10)-C(9)-H(9B)	109.0
H(9A)-C(9)-H(9B)	107.8	C(5)-C(10)-C(9)	111.1(3)
C(5)-C(10)-H(10A)	109.4	C(9)-C(10)-H(10A)	109.4
C(5)-C(10)-H(10B)	109.4	C(9)-C(10)-H(10B)	109.4
H(10A)-C(10)-H(10B)	108.0	N(2)-C(11)-C(12)	109.4(2)
N(2)-C(11)-C(16)	112.1(2)	C(12)-C(11)-C(16)	111.9(2)
N(2)-C(11)-H(11)	107.8	C(12)-C(11)-H(11)	107.8
C(16)-C(11)-H(11)	107.8	C(13)-C(12)-C(11)	110.6(2)
C(13)-C(12)-H(12A)	109.5	C(11)-C(12)-H(12A)	109.5
C(13)-C(12)-H(12B)	109.5	C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1	C(12)-C(13)-C(14)	111.4(3)
C(12)-C(13)-H(13A)	109.3	C(14)-C(13)-H(13A)	109.3
C(12)-C(13)-H(13B)	109.3	C(14)-C(13)-H(13B)	109.3
H(13A)-C(13)-H(13B)	108.0	C(13)-C(14)-C(15)	110.3(3)
C(13)-C(14)-H(14A)	109.6	C(15)-C(14)-H(14A)	109.6
C(13)-C(14)-H(14B)	109.6	C(15)-C(14)-H(14B)	109.6
H(14A)-C(14)-H(14B)	108.1	C(14)-C(15)-C(16)	111.3(3)
C(14)-C(15)-H(15A)	109.4	C(16)-C(15)-H(15A)	109.4
C(14)-C(15)-H(15B)	109.4	C(16)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0	C(11)-C(16)-C(15)	110.1(2)
C(11)-C(16)-H(16A)	109.6	C(15)-C(16)-H(16A)	109.6
C(11)-C(16)-H(16B)	109.6	C(15)-C(16)-H(16B)	109.6
H(16A)-C(16)-H(16B)	108.2	C(18)-C(17)-C(22)	111.7(3)
C(18)-C(17)-Ru(1)	124.1(2)	C(22)-C(17)-Ru(1)	124.2(2)
F(5)-C(18)-C(17)	120.9(3)	F(5)-C(18)-C(19)	114.1(3)
C(17)-C(18)-C(19)	125.0(3)	F(4)-C(19)-C(20)	121.0(3)
F(4)-C(19)-C(18)	120.0(4)	C(20)-C(19)-C(18)	119.0(4)
C(21)-C(20)-F(3)	121.5(4)	C(21)-C(20)-C(19)	119.0(3)
F(3)-C(20)-C(19)	119.5(4)	C(20)-C(21)-F(2)	119.4(3)
C(20)-C(21)-C(22)	120.1(4)	F(2)-C(21)-C(22)	120.5(4)
F(1)-C(22)-C(21)	114.0(3)	F(1)-C(22)-C(17)	120.8(3)
C(21)-C(22)-C(17)	125.2(4)	C(24)-C(23)-C(28)	117.8(3)
C(24)-C(23)-P(1)	118.9(2)	C(28)-C(23)-P(1)	123.1(2)
C(25)-C(24)-C(23)	121.7(3)	C(25)-C(24)-H(24)	119.2
C(23)-C(24)-H(24)	119.2	C(24)-C(25)-C(26)	119.6(3)
C(24)-C(25)-H(25)	120.2	C(26)-C(25)-H(25)	120.2
C(27)-C(26)-C(25)	119.9(3)	C(27)-C(26)-H(26)	120.0
C(25)-C(26)-H(26)	120.0	C(26)-C(27)-C(28)	120.4(3)
C(26)-C(27)-H(27)	119.8	C(28)-C(27)-H(27)	119.8
C(27)-C(28)-C(23)	120.6(3)	C(27)-C(28)-H(28)	119.7
C(23)-C(28)-H(28)	119.7	C(30)-C(29)-C(34)	118.2(3)
C(30)-C(29)-P(1)	119.1(2)	C(34)-C(29)-P(1)	122.4(2)
C(29)-C(30)-C(31)	120.5(3)	C(29)-C(30)-H(30)	119.8
C(31)-C(30)-H(30)	119.8	C(32)-C(31)-C(30)	119.9(3)
C(32)-C(31)-H(31)	120.1	C(30)-C(31)-H(31)	120.1
C(31)-C(32)-C(33)	120.3(3)	C(31)-C(32)-H(32)	119.8
C(33)-C(32)-H(32)	119.8	C(32)-C(33)-C(34)	120.1(3)
C(32)-C(33)-H(33)	120.0	C(34)-C(33)-H(33)	120.0
C(33)-C(34)-C(29)	121.0(3)	C(33)-C(34)-H(34)	119.5
C(29)-C(34)-H(34)	119.5	C(36)-C(35)-P(1)	114.16(19)
C(36)-C(35)-H(35A)	108.7	P(1)-C(35)-H(35A)	108.7
C(36)-C(35)-H(35B)	108.7	P(1)-C(35)-H(35B)	108.7
H(35A)-C(35)-H(35B)	107.6	C(37)-C(36)-C(35)	113.4(2)
C(37)-C(36)-H(36A)	108.9	C(35)-C(36)-H(36A)	108.9
C(37)-C(36)-H(36B)	108.9	C(35)-C(36)-H(36B)	108.9

H(36A)-C(36)-H(36B)	107.7	C(36)-C(37)-P(2)	113.40(19)
C(36)-C(37)-H(37A)	108.9	P(2)-C(37)-H(37A)	108.9
C(36)-C(37)-H(37B)	108.9	P(2)-C(37)-H(37B)	108.9
H(37A)-C(37)-H(37B)	107.7	C(43)-C(38)-C(39)	118.1(3)
C(43)-C(38)-P(2)	122.4(2)	C(39)-C(38)-P(2)	119.4(2)
C(40)-C(39)-C(38)	121.3(3)	C(40)-C(39)-H(39)	119.3
C(38)-C(39)-H(39)	119.3	C(39)-C(40)-C(41)	119.9(3)
C(39)-C(40)-H(40)	120.0	C(41)-C(40)-H(40)	120.0
C(42)-C(41)-C(40)	119.7(3)	C(42)-C(41)-H(41)	120.2
C(40)-C(41)-H(41)	120.2	C(41)-C(42)-C(43)	120.4(3)
C(41)-C(42)-H(42)	119.8	C(43)-C(42)-H(42)	119.8
C(38)-C(43)-C(42)	120.5(3)	C(38)-C(43)-H(43)	119.8
C(42)-C(43)-H(43)	119.8	C(45)-C(44)-C(49)	117.8(3)
C(45)-C(44)-P(2)	122.2(2)	C(49)-C(44)-P(2)	119.7(2)
C(46)-C(45)-C(44)	120.6(3)	C(46)-C(45)-H(45)	119.7
C(44)-C(45)-H(45)	119.7	C(47)-C(46)-C(45)	121.1(3)
C(47)-C(46)-H(46)	119.5	C(45)-C(46)-H(46)	119.5
C(46)-C(47)-C(48)	118.8(3)	C(46)-C(47)-H(47)	120.6
C(48)-C(47)-H(47)	120.6	C(49)-C(48)-C(47)	120.7(3)
C(49)-C(48)-H(48)	119.7	C(47)-C(48)-H(48)	119.7
C(48)-C(49)-C(44)	121.1(3)	C(48)-C(49)-H(49)	119.5
C(44)-C(49)-H(49)	119.5		

Table 126. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(ICy)(dppp)(CO)(C_6F_5)H **(80)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	17(1)	19(1)	20(1)	-2(1)	-8(1)	2(1)
P(1)	17(1)	21(1)	19(1)	-3(1)	-8(1)	2(1)
P(2)	16(1)	21(1)	20(1)	-2(1)	-7(1)	2(1)
F(1)	44(1)	30(1)	67(1)	8(1)	-25(1)	-11(1)
F(2)	51(1)	32(1)	139(2)	-26(1)	-43(2)	-3(1)
F(3)	74(2)	85(2)	153(3)	-86(2)	-60(2)	15(1)
F(4)	65(2)	117(2)	63(2)	-62(2)	-34(1)	19(1)
F(5)	39(1)	61(1)	29(1)	-16(1)	-16(1)	5(1)
O(1)	39(1)	30(1)	24(1)	3(1)	-10(1)	0(1)
N(1)	21(1)	27(1)	26(1)	1(1)	-8(1)	5(1)
N(2)	23(1)	26(1)	24(1)	3(1)	-6(1)	9(1)
C(1)	21(2)	25(2)	24(2)	-9(1)	-11(1)	7(1)
C(2)	22(2)	22(2)	21(2)	-5(1)	-13(1)	6(1)
C(3)	29(2)	49(2)	34(2)	12(2)	-6(2)	20(2)
C(4)	32(2)	51(2)	36(2)	8(2)	-4(2)	24(2)
C(5)	21(2)	35(2)	24(2)	1(1)	-7(1)	8(1)
C(6)	58(2)	70(3)	31(2)	16(2)	-24(2)	-34(2)
C(7)	54(3)	138(4)	38(2)	30(3)	-19(2)	-45(3)
C(8)	38(2)	80(3)	28(2)	13(2)	-10(2)	-6(2)
C(9)	74(3)	49(2)	32(2)	-11(2)	-30(2)	31(2)
C(10)	50(2)	31(2)	36(2)	9(2)	-23(2)	-8(2)
C(11)	23(2)	25(2)	20(2)	-2(1)	-6(1)	6(1)
C(12)	34(2)	36(2)	23(2)	0(1)	-10(1)	-5(2)
C(13)	35(2)	35(2)	26(2)	1(1)	-6(2)	-4(2)
C(14)	44(2)	43(2)	24(2)	0(2)	-4(2)	7(2)
C(15)	61(2)	42(2)	30(2)	-15(2)	-16(2)	8(2)

C(16)	37(2)	27(2)	39(2)	-8(1)	-12(2)	0(2)
C(17)	16(1)	22(2)	35(2)	-14(1)	-14(1)	10(1)
C(18)	23(2)	39(2)	47(2)	-20(2)	-17(2)	9(2)
C(19)	38(2)	71(3)	55(2)	-47(2)	-28(2)	24(2)
C(20)	41(2)	51(3)	104(4)	-56(3)	-40(2)	16(2)
C(21)	32(2)	28(2)	99(3)	-28(2)	-30(2)	6(2)
C(22)	22(2)	27(2)	71(3)	-14(2)	-22(2)	8(1)
C(23)	19(1)	27(2)	19(1)	-7(1)	-10(1)	0(1)
C(24)	21(2)	31(2)	25(2)	-5(1)	-10(1)	2(1)
C(25)	20(2)	34(2)	27(2)	-9(1)	-13(1)	5(1)
C(26)	16(2)	44(2)	27(2)	-14(1)	-8(1)	-1(1)
C(27)	26(2)	33(2)	23(2)	-1(1)	-10(1)	-7(1)
C(28)	27(2)	28(2)	24(2)	-3(1)	-14(1)	3(1)
C(29)	23(2)	23(2)	23(2)	-4(1)	-9(1)	5(1)
C(30)	30(2)	29(2)	26(2)	-5(1)	-11(1)	5(1)
C(31)	38(2)	36(2)	26(2)	-4(2)	-2(2)	7(2)
C(32)	58(2)	45(2)	22(2)	-11(2)	-16(2)	16(2)
C(33)	48(2)	49(2)	30(2)	-15(2)	-19(2)	6(2)
C(34)	35(2)	35(2)	28(2)	-7(1)	-14(2)	2(2)
C(35)	24(2)	21(2)	23(2)	-7(1)	-10(1)	3(1)
C(36)	23(2)	20(2)	28(2)	-4(1)	-10(1)	4(1)
C(37)	17(1)	21(2)	28(2)	-2(1)	-8(1)	3(1)
C(38)	19(2)	24(2)	19(1)	-5(1)	-8(1)	-1(1)
C(39)	23(2)	30(2)	26(2)	-6(1)	-11(1)	3(1)
C(40)	20(2)	41(2)	27(2)	-14(1)	-6(1)	5(1)
C(41)	24(2)	46(2)	24(2)	-9(2)	-1(1)	-6(2)
C(42)	34(2)	39(2)	28(2)	5(2)	-9(2)	-5(2)
C(43)	23(2)	34(2)	29(2)	-3(1)	-9(1)	0(1)
C(44)	16(1)	25(2)	21(2)	-5(1)	-8(1)	6(1)
C(45)	22(2)	28(2)	25(2)	0(1)	-9(1)	2(1)
C(46)	29(2)	44(2)	19(2)	0(1)	-9(1)	5(2)
C(47)	29(2)	47(2)	27(2)	-14(2)	-16(2)	9(2)
C(48)	24(2)	35(2)	34(2)	-10(1)	-14(2)	2(1)
C(49)	21(2)	30(2)	23(2)	-4(1)	-11(1)	5(1)

Table 127. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(ICy)(dppp)(CO)(C_6F_5)H **(80)**.

Atom	x	y	z	U(eq)
H(3)	5237	103	3418	50
H(4)	6281	551	1514	53
H(5)	2557	1496	4541	33
H(6A)	3257	-478	4621	63
H(6B)	2258	-95	4230	63
H(7A)	1384	-807	5996	95
H(7B)	1085	322	5931	95
H(8A)	1676	-36	7336	61
H(8B)	2870	-490	6579	61
H(9A)	3299	1075	6806	59
H(9B)	2280	1509	6472	59
H(10A)	4079	1860	5051	46
H(10B)	4430	743	5085	46
H(11)	4682	2408	530	28
H(12A)	6146	3162	872	38

H(12B)	7022	2296	447	38
H(13A)	7504	3597	-886	41
H(13B)	6180	3617	-807	41
H(14A)	7772	2076	-1538	49
H(14B)	7342	2823	-2265	49
H(15A)	6269	1320	-1842	53
H(15B)	5404	2189	-1405	53
H(16A)	4906	873	-76	42
H(16B)	6231	834	-157	42
H(24)	5104	2832	3547	30
H(25)	7141	2980	2806	31
H(26)	8067	4301	1562	34
H(27)	6945	5459	1079	33
H(28)	4897	5317	1825	30
H(30)	1219	3056	5161	34
H(31)	648	3005	6985	44
H(32)	1910	3619	7649	50
H(33)	3716	4323	6513	48
H(34)	4266	4428	4706	38
H(35A)	2894	5501	3548	27
H(35B)	3006	5323	2400	27
H(36A)	929	4706	4201	28
H(36B)	1062	5791	3638	28
H(37A)	1349	5072	2026	27
H(37B)	41	5004	2912	27
H(39)	-1557	4055	3522	31
H(40)	-3297	3599	4951	35
H(41)	-3300	2393	6259	40
H(42)	-1556	1648	6120	43
H(43)	176	2037	4630	35
H(45)	1129	4464	696	30
H(46)	611	4115	-661	37
H(47)	-493	2721	-496	38
H(48)	-1117	1679	1074	36
H(49)	-629	2021	2439	29
H(1)	1857(19)	2074(15)	3593(10)	18(7)

Table 128. Dihedral angles [°] for Ru(ICy)(dppp)(CO)(C_6F_5)H **(80)**.

Atom1 - Atom2 - Atom3 - Atom4	Dihedral
C(1) - Ru(1) - P(1) - C(29)	178.34(14)
C(2) - Ru(1) - P(1) - C(29)	-79.38(13)
C(17) - Ru(1) - P(1) - C(29)	-94.0(19)
P(2) - Ru(1) - P(1) - C(29)	88.80(11)
C(1) - Ru(1) - P(1) - C(23)	-58.39(13)
C(2) - Ru(1) - P(1) - C(23)	43.89(12)
C(17) - Ru(1) - P(1) - C(23)	29.3(19)
P(2) - Ru(1) - P(1) - C(23)	-147.93(10)
C(1) - Ru(1) - P(1) - C(35)	57.75(13)
C(2) - Ru(1) - P(1) - C(35)	160.04(12)
C(17) - Ru(1) - P(1) - C(35)	145.4(19)
P(2) - Ru(1) - P(1) - C(35)	-31.78(10)
C(1) - Ru(1) - P(2) - C(44)	66.13(13)
C(2) - Ru(1) - P(2) - C(44)	-91.7(3)

C(17) - Ru(1) - P(2) - C(44)	-30.02(12)
P(1) - Ru(1) - P(2) - C(44)	149.86(10)
C(1) - Ru(1) - P(2) - C(37)	-52.47(13)
C(2) - Ru(1) - P(2) - C(37)	149.7(3)
C(17) - Ru(1) - P(2) - C(37)	-148.62(13)
P(1) - Ru(1) - P(2) - C(37)	31.26(10)
C(1) - Ru(1) - P(2) - C(38)	-174.36(13)
C(2) - Ru(1) - P(2) - C(38)	27.8(3)
C(17) - Ru(1) - P(2) - C(38)	89.49(13)
P(1) - Ru(1) - P(2) - C(38)	-90.63(10)
C(2) - Ru(1) - C(1) - O(1)	-133.0(14)
C(17) - Ru(1) - C(1) - O(1)	140.8(14)
P(2) - Ru(1) - C(1) - O(1)	52.2(14)
P(1) - Ru(1) - C(1) - O(1)	-41.6(14)
C(4) - N(2) - C(2) - N(1)	-0.8(3)
C(11) - N(2) - C(2) - N(1)	-175.8(2)
C(4) - N(2) - C(2) - Ru(1)	-175.1(2)
C(11) - N(2) - C(2) - Ru(1)	10.0(4)
C(3) - N(1) - C(2) - N(2)	0.3(3)
C(5) - N(1) - C(2) - N(2)	-176.2(3)
C(3) - N(1) - C(2) - Ru(1)	174.4(2)
C(5) - N(1) - C(2) - Ru(1)	-2.0(4)
C(1) - Ru(1) - C(2) - N(2)	-26.8(3)
C(17) - Ru(1) - C(2) - N(2)	68.4(2)
P(2) - Ru(1) - C(2) - N(2)	130.5(3)
P(1) - Ru(1) - C(2) - N(2)	-111.0(2)
C(1) - Ru(1) - C(2) - N(1)	160.4(2)
C(17) - Ru(1) - C(2) - N(1)	-104.4(3)
P(2) - Ru(1) - C(2) - N(1)	-42.3(5)
P(1) - Ru(1) - C(2) - N(1)	76.2(2)
C(2) - N(1) - C(3) - C(4)	0.4(4)
C(5) - N(1) - C(3) - C(4)	177.2(3)
N(1) - C(3) - C(4) - N(2)	-0.9(4)
C(2) - N(2) - C(4) - C(3)	1.1(4)
C(11) - N(2) - C(4) - C(3)	176.3(3)
C(3) - N(1) - C(5) - C(6)	-62.9(4)
C(2) - N(1) - C(5) - C(6)	113.3(3)
C(3) - N(1) - C(5) - C(10)	59.6(4)
C(2) - N(1) - C(5) - C(10)	-124.2(3)
N(1) - C(5) - C(6) - C(7)	-177.4(3)
C(10) - C(5) - C(6) - C(7)	58.3(4)
C(5) - C(6) - C(7) - C(8)	-58.8(5)
C(6) - C(7) - C(8) - C(9)	55.4(5)
C(7) - C(8) - C(9) - C(10)	-54.0(4)
N(1) - C(5) - C(10) - C(9)	-177.8(2)
C(6) - C(5) - C(10) - C(9)	-55.2(4)
C(8) - C(9) - C(10) - C(5)	54.5(4)
C(2) - N(2) - C(11) - C(12)	103.2(3)
C(4) - N(2) - C(11) - C(12)	-71.3(4)
C(2) - N(2) - C(11) - C(16)	-132.1(3)
C(4) - N(2) - C(11) - C(16)	53.4(4)
N(2) - C(11) - C(12) - C(13)	-179.2(2)
C(16) - C(11) - C(12) - C(13)	55.9(3)
C(11) - C(12) - C(13) - C(14)	-56.2(4)
C(12) - C(13) - C(14) - C(15)	56.7(4)

C(13) - C(14) - C(15) - C(16)	-56.8(4)
N(2) - C(11) - C(16) - C(15)	-179.2(3)
C(12) - C(11) - C(16) - C(15)	-55.8(3)
C(14) - C(15) - C(16) - C(11)	56.1(4)
C(1) - Ru(1) - C(17) - C(18)	-0.6(3)
C(2) - Ru(1) - C(17) - C(18)	-102.7(2)
P(2) - Ru(1) - C(17) - C(18)	89.2(2)
P(1) - Ru(1) - C(17) - C(18)	-88.0(19)
C(1) - Ru(1) - C(17) - C(22)	178.4(2)
C(2) - Ru(1) - C(17) - C(22)	76.4(2)
P(2) - Ru(1) - C(17) - C(22)	-91.8(2)
P(1) - Ru(1) - C(17) - C(22)	91.1(19)
C(22) - C(17) - C(18) - F(5)	180.0(3)
Ru(1) - C(17) - C(18) - F(5)	-0.9(4)
C(22) - C(17) - C(18) - C(19)	0.8(4)
Ru(1) - C(17) - C(18) - C(19)	179.9(2)
F(5) - C(18) - C(19) - F(4)	0.9(4)
C(17) - C(18) - C(19) - F(4)	-179.8(3)
F(5) - C(18) - C(19) - C(20)	-179.2(3)
C(17) - C(18) - C(19) - C(20)	0.0(5)
F(4) - C(19) - C(20) - C(21)	179.8(3)
C(18) - C(19) - C(20) - C(21)	0.0(5)
F(4) - C(19) - C(20) - F(3)	0.6(5)
C(18) - C(19) - C(20) - F(3)	-179.3(3)
F(3) - C(20) - C(21) - F(2)	-0.1(5)
C(19) - C(20) - C(21) - F(2)	-179.3(3)
F(3) - C(20) - C(21) - C(22)	178.4(3)
C(19) - C(20) - C(21) - C(22)	-0.8(6)
C(20) - C(21) - C(22) - F(1)	179.4(3)
F(2) - C(21) - C(22) - F(1)	-2.1(4)
C(20) - C(21) - C(22) - C(17)	1.8(5)
F(2) - C(21) - C(22) - C(17)	-179.7(3)
C(18) - C(17) - C(22) - F(1)	-179.1(3)
Ru(1) - C(17) - C(22) - F(1)	1.7(4)
C(18) - C(17) - C(22) - C(21)	-1.7(4)
Ru(1) - C(17) - C(22) - C(21)	179.2(2)
C(29) - P(1) - C(23) - C(24)	57.9(2)
C(35) - P(1) - C(23) - C(24)	160.5(2)
Ru(1) - P(1) - C(23) - C(24)	-76.7(2)
C(29) - P(1) - C(23) - C(28)	-127.4(2)
C(35) - P(1) - C(23) - C(28)	-24.8(3)
Ru(1) - P(1) - C(23) - C(28)	98.0(2)
C(28) - C(23) - C(24) - C(25)	0.5(4)
P(1) - C(23) - C(24) - C(25)	175.4(2)
C(23) - C(24) - C(25) - C(26)	-0.4(4)
C(24) - C(25) - C(26) - C(27)	0.1(4)
C(25) - C(26) - C(27) - C(28)	0.0(4)
C(26) - C(27) - C(28) - C(23)	0.1(4)
C(24) - C(23) - C(28) - C(27)	-0.4(4)
P(1) - C(23) - C(28) - C(27)	-175.1(2)
C(23) - P(1) - C(29) - C(30)	-163.2(2)
C(35) - P(1) - C(29) - C(30)	92.0(2)
Ru(1) - P(1) - C(29) - C(30)	-35.0(3)
C(23) - P(1) - C(29) - C(34)	22.2(3)
C(35) - P(1) - C(29) - C(34)	-82.5(3)

Ru(1) - P(1) - C(29) - C(34)	150.4(2)
C(34) - C(29) - C(30) - C(31)	-0.8(4)
P(1) - C(29) - C(30) - C(31)	-175.6(2)
C(29) - C(30) - C(31) - C(32)	-0.7(5)
C(30) - C(31) - C(32) - C(33)	1.0(5)
C(31) - C(32) - C(33) - C(34)	0.1(5)
C(32) - C(33) - C(34) - C(29)	-1.7(5)
C(30) - C(29) - C(34) - C(33)	2.0(5)
P(1) - C(29) - C(34) - C(33)	176.6(2)
C(29) - P(1) - C(35) - C(36)	-77.2(2)
C(23) - P(1) - C(35) - C(36)	178.41(19)
Ru(1) - P(1) - C(35) - C(36)	56.1(2)
P(1) - C(35) - C(36) - C(37)	-78.1(3)
C(35) - C(36) - C(37) - P(2)	75.7(3)
C(44) - P(2) - C(37) - C(36)	-178.02(19)
C(38) - P(2) - C(37) - C(36)	78.7(2)
Ru(1) - P(2) - C(37) - C(36)	-53.5(2)
C(44) - P(2) - C(38) - C(43)	123.9(2)
C(37) - P(2) - C(38) - C(43)	-130.8(2)
Ru(1) - P(2) - C(38) - C(43)	-2.0(3)
C(44) - P(2) - C(38) - C(39)	-53.7(2)
C(37) - P(2) - C(38) - C(39)	51.5(2)
Ru(1) - P(2) - C(38) - C(39)	-179.67(18)
C(43) - C(38) - C(39) - C(40)	-0.3(4)
P(2) - C(38) - C(39) - C(40)	177.5(2)
C(38) - C(39) - C(40) - C(41)	1.4(4)
C(39) - C(40) - C(41) - C(42)	-0.3(5)
C(40) - C(41) - C(42) - C(43)	-1.8(5)
C(39) - C(38) - C(43) - C(42)	-1.8(4)
P(2) - C(38) - C(43) - C(42)	-179.5(2)
C(41) - C(42) - C(43) - C(38)	2.9(5)
C(37) - P(2) - C(44) - C(45)	39.6(3)
C(38) - P(2) - C(44) - C(45)	143.2(2)
Ru(1) - P(2) - C(44) - C(45)	-86.2(2)
C(37) - P(2) - C(44) - C(49)	-147.6(2)
C(38) - P(2) - C(44) - C(49)	-44.0(2)
Ru(1) - P(2) - C(44) - C(49)	86.7(2)
C(49) - C(44) - C(45) - C(46)	-0.3(4)
P(2) - C(44) - C(45) - C(46)	172.6(2)
C(44) - C(45) - C(46) - C(47)	-0.3(5)
C(45) - C(46) - C(47) - C(48)	0.7(5)
C(46) - C(47) - C(48) - C(49)	-0.3(5)
C(47) - C(48) - C(49) - C(44)	-0.4(4)
C(45) - C(44) - C(49) - C(48)	0.7(4)
P(2) - C(44) - C(49) - C(48)	-172.5(2)

Table 129. Crystal data and structure refinement for Ru(ICy)(dppp)(CO)($C_6F_4CF_3$)H **(81)**.

Compound	Ru(ICy)(dppp)(CO)($C_6F_4CF_3$)H **(81)**
Empirical formula	C56 H55 F7 N2 O P2 Ru
Formula weight	1068.03
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P-1
Unit cell dimensions	a = 13.5440(2)Å α = 64.739(1)^o
	b = 13.5560(2)Å β = 87.984(1)^o
	c = 15.1060(2)Å γ = 81.794(1)^o
Volume	2481.57(6) Å^3
Z	2
Density (calculated)	1.429 Mg/m^3
Absorption coefficient	0.449 mm^{-1}
F(000)	1100
Crystal size	0.22 x 0.15 x 0.15 mm
Theta range for data collection	3.84 to 27.51^o
Index ranges	-17<=h<=17; -16<=k<=17; -19<=l<=19
Reflections collected	44147
Independent reflections	11348 [R(int) = 0.0644]
Reflections observed (>2σ)	8898
Data Completeness	0.994
Absorption correction	PSI-Scans
Max. and min. transmission	0.94 and 0.87
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11348 / 1 / 654
Goodness-of-fit on F^2	1.024
Final R indices [I>2σ(I)]	R1 = 0.0376 wR2 = 0.0861
R indices (all data)	R1 = 0.0578 wR2 = 0.0938
Largest diff. peak and hole	0.829 and -0.780 eÅ^{-3}

Table 130. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Ru(ICy)(dppp)(CO)($C_6F_4CF_3$)H **(81)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	7609(1)	2521(1)	7817(1)	18(1)
P(1)	6216(1)	1691(1)	8506(1)	19(1)
P(2)	7756(1)	3037(1)	9077(1)	21(1)
F(1)	8358(1)	341(1)	7325(1)	33(1)
F(2)	7844(1)	-255(1)	6009(1)	44(1)
F(3)	5901(1)	3230(1)	4318(1)	38(1)
F(4)	6382(1)	3843(1)	5618(1)	32(1)
F(5)	6043(6)	1811(7)	3625(7)	70(2)
F(5A)	6311(17)	1887(18)	3516(15)	135(8)
F(6)	6070(7)	214(5)	4796(7)	70(2)
F(6A)	5766(14)	605(14)	4580(12)	124(7)
F(7)	7361(7)	678(11)	4024(8)	65(2)
F(7A)	7260(17)	450(20)	4200(18)	123(9)
O(1)	8833(1)	350(1)	9187(1)	33(1)
N(1)	8534(1)	4716(2)	6493(1)	27(1)

N(2)	9698(1)	3330(2)	7015(1)	25(1)
C(1)	8436(2)	1167(2)	8610(2)	24(1)
C(2)	7383(2)	2136(2)	6597(2)	20(1)
C(3)	7730(2)	1106(2)	6597(2)	26(1)
C(4)	7471(2)	776(2)	5906(2)	31(1)
C(5)	6848(2)	1453(2)	5111(2)	31(1)
C(6)	6505(2)	2490(2)	5068(2)	28(1)
C(7)	6778(2)	2794(2)	5779(2)	25(1)
C(8)	6573(2)	1067(2)	4378(2)	44(1)
C(9)	8683(2)	3581(2)	7033(2)	21(1)
C(10)	9425(2)	5112(2)	6182(2)	34(1)
C(11)	10148(2)	4259(2)	6500(2)	33(1)
C(12)	7577(2)	5466(2)	6173(2)	28(1)
C(13)	7466(2)	5947(2)	5056(2)	34(1)
C(14)	6483(2)	6719(2)	4699(2)	42(1)
C(15)	6409(2)	7640(2)	5032(2)	42(1)
C(16)	6549(2)	7175(2)	6134(2)	41(1)
C(17)	7530(2)	6394(2)	6497(2)	35(1)
C(18)	10267(2)	2207(2)	7407(2)	27(1)
C(19)	10304(2)	1762(2)	6641(2)	37(1)
C(20)	10869(2)	583(2)	7048(2)	45(1)
C(21)	11908(2)	541(2)	7419(2)	38(1)
C(22)	11861(2)	1017(2)	8172(2)	41(1)
C(23)	11314(2)	2186(2)	7753(2)	33(1)
C(24)	6296(2)	956(2)	9850(2)	24(1)
C(25)	6420(2)	1694(2)	10362(2)	26(1)
C(26)	7471(2)	2005(2)	10298(2)	26(1)
C(27)	4979(2)	2542(2)	8287(2)	21(1)
C(28)	4224(2)	2215(2)	8956(2)	28(1)
C(29)	3283(2)	2827(2)	8771(2)	33(1)
C(30)	3083(2)	3778(2)	7920(2)	34(1)
C(31)	3818(2)	4112(2)	7242(2)	35(1)
C(32)	4763(2)	3493(2)	7425(2)	28(1)
C(33)	5941(2)	590(2)	8186(2)	22(1)
C(34)	5164(2)	760(2)	7535(2)	28(1)
C(35)	5007(2)	-65(2)	7266(2)	34(1)
C(36)	5615(2)	-1069(2)	7646(2)	34(1)
C(37)	6389(2)	-1244(2)	8289(2)	34(1)
C(38)	6555(2)	-421(2)	8553(2)	28(1)
C(39)	6974(2)	4257(2)	9092(2)	26(1)
C(40)	7148(2)	4633(2)	9797(2)	35(1)
C(41)	6500(2)	5491(2)	9854(2)	45(1)
C(42)	5682(2)	5980(2)	9224(2)	44(1)
C(43)	5501(2)	5621(2)	8531(2)	38(1)
C(44)	6146(2)	4759(2)	8461(2)	29(1)
C(45)	9017(2)	3235(2)	9329(2)	27(1)
C(46)	9695(2)	2347(2)	9930(2)	35(1)
C(47)	10634(2)	2501(3)	10147(2)	43(1)
C(48)	10903(2)	3544(3)	9758(2)	48(1)
C(49)	10256(2)	4420(3)	9129(2)	49(1)
C(50)	9315(2)	4270(2)	8913(2)	37(1)
C(51)	9835(3)	2042(3)	3974(3)	75(1)
C(52)	9064(3)	2701(3)	4137(3)	68(1)
C(53)	8346(3)	3300(3)	3435(3)	67(1)
C(54)	8374(3)	3229(3)	2567(3)	75(1)

C(55)	9151(3)	2574(3)	2379(3)	74(1)
C(56)	9889(3)	1991(3)	3076(4)	80(1)

Table 131. Bond lengths [Å] and angles [°] for Ru(ICy)(dppp)(CO)($C_6F_4CF_3$)H **(81)**.

Ru(1)-C(1)	1.921(2)	Ru(1)-C(9)	2.145(2)
Ru(1)-C(2)	2.160(2)	Ru(1)-P(2)	2.3150(6)
Ru(1)-P(1)	2.3191(6)	Ru(1)-H(1)	1.599(5)
P(1)-C(24)	1.839(2)	P(1)-C(33)	1.841(2)
P(1)-C(27)	1.846(2)	P(2)-C(39)	1.841(2)
P(2)-C(45)	1.843(2)	P(2)-C(26)	1.846(2)
F(1)-C(3)	1.360(3)	F(2)-C(4)	1.360(3)
F(3)-C(6)	1.349(3)	F(4)-C(7)	1.365(2)
F(5)-C(8)	1.303(8)	F(5A)-C(8)	1.32(2)
F(6)-C(8)	1.332(9)	F(6A)-C(8)	1.300(17)
F(7)-C(8)	1.320(10)	F(7A)-C(8)	1.26(2)
O(1)-C(1)	1.146(3)	N(1)-C(10)	1.377(3)
N(1)-C(9)	1.387(3)	N(1)-C(12)	1.482(3)
N(2)-C(9)	1.372(3)	N(2)-C(11)	1.381(3)
N(2)-C(18)	1.480(3)	C(2)-C(7)	1.384(3)
C(2)-C(3)	1.409(3)	C(3)-C(4)	1.372(3)
C(4)-C(5)	1.379(3)	C(5)-C(6)	1.391(3)
C(5)-C(8)	1.489(3)	C(6)-C(7)	1.383(3)
C(10)-C(11)	1.327(3)	C(10)-H(10)	0.9500
C(11)-H(11)	0.9500	C(12)-C(17)	1.525(3)
C(12)-C(13)	1.531(3)	C(13)-C(14)	1.526(3)
C(13)-H(13A)	0.9900	C(13)-H(13B)	0.9900
C(14)-C(15)	1.523(4)	C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900	C(15)-C(16)	1.515(4)
C(15)-H(15A)	0.9900	C(15)-H(15B)	0.9900
C(16)-C(17)	1.531(3)	C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900	C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900	C(18)-C(19)	1.513(3)
C(18)-C(23)	1.521(3)	C(19)-C(20)	1.537(3)
C(19)-H(19A)	0.9900	C(19)-H(19B)	0.9900
C(20)-C(21)	1.518(4)	C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900	C(21)-C(22)	1.524(4)
C(21)-H(21A)	0.9900	C(21)-H(21B)	0.9900
C(22)-C(23)	1.517(3)	C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900	C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900	C(24)-C(25)	1.531(3)
C(24)-H(24B)	0.9900	C(24)-H(24A)	0.9900
C(25)-C(26)	1.530(3)	C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900	C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900	C(27)-C(32)	1.389(3)
C(27)-C(28)	1.393(3)	C(28)-C(29)	1.384(3)
C(28)-H(28)	0.9500	C(29)-C(30)	1.378(4)
C(29)-H(29)	0.9500	C(30)-C(31)	1.381(4)
C(30)-H(30)	0.9500	C(31)-C(32)	1.392(3)
C(31)-H(31)	0.9500	C(32)-H(32)	0.9500
C(33)-C(38)	1.391(3)	C(33)-C(34)	1.392(3)
C(34)-C(35)	1.385(3)	C(34)-H(34)	0.9500
C(35)-C(36)	1.381(3)	C(35)-H(35)	0.9500
C(36)-C(37)	1.379(4)	C(36)-H(36)	0.9500
C(37)-C(38)	1.382(3)	C(37)-H(37)	0.9500

C(38)-H(38)	0.9500	C(39)-C(44)	1.391(3)
C(39)-C(40)	1.401(3)	C(40)-C(41)	1.385(4)
C(40)-H(40)	0.9500	C(41)-C(42)	1.377(4)
C(41)-H(41)	0.9500	C(42)-C(43)	1.372(4)
C(42)-H(42)	0.9500	C(43)-C(44)	1.395(3)
C(43)-H(43)	0.9500	C(44)-H(44)	0.9500
C(45)-C(50)	1.385(3)	C(45)-C(46)	1.387(3)
C(46)-C(47)	1.389(4)	C(46)-H(46)	0.9500
C(47)-C(48)	1.379(4)	C(47)-H(47)	0.9500
C(48)-C(49)	1.372(4)	C(48)-H(48)	0.9500
C(49)-C(50)	1.391(4)	C(49)-H(49)	0.9500
C(50)-H(50)	0.9500	C(51)-C(52)	1.360(5)
C(51)-C(56)	1.386(6)	C(51)-H(51)	0.9500
C(52)-C(53)	1.358(5)	C(52)-H(52)	0.9500
C(53)-C(54)	1.353(5)	C(53)-H(53)	0.9500
C(54)-C(55)	1.380(5)	C(54)-H(54)	0.9500
C(55)-C(56)	1.369(5)	C(55)-H(55)	0.9500
C(56)-H(56)	0.9500		
C(1)-Ru(1)-C(9)	102.65(9)	C(1)-Ru(1)-C(2)	97.01(9)
C(9)-Ru(1)-C(2)	91.66(8)	C(1)-Ru(1)-P(2)	87.05(7)
C(9)-Ru(1)-P(2)	88.49(6)	C(2)-Ru(1)-P(2)	175.80(6)
C(1)-Ru(1)-P(1)	88.92(7)	C(9)-Ru(1)-P(1)	168.40(6)
C(2)-Ru(1)-P(1)	87.72(6)	P(2)-Ru(1)-P(1)	91.29(2)
C(1)-Ru(1)-H(1)	173.7(8)	C(9)-Ru(1)-H(1)	82.7(8)
C(2)-Ru(1)-H(1)	86.0(8)	P(2)-Ru(1)-H(1)	89.8(8)
P(1)-Ru(1)-H(1)	85.7(8)	C(24)-P(1)-C(33)	100.55(10)
C(24)-P(1)-C(27)	102.38(10)	C(33)-P(1)-C(27)	100.76(10)
C(24)-P(1)-Ru(1)	113.97(8)	C(33)-P(1)-Ru(1)	116.86(7)
C(27)-P(1)-Ru(1)	119.54(7)	C(39)-P(2)-C(45)	102.52(10)
C(39)-P(2)-C(26)	98.88(10)	C(45)-P(2)-C(26)	100.12(11)
C(39)-P(2)-Ru(1)	121.28(8)	C(45)-P(2)-Ru(1)	116.12(7)
C(26)-P(2)-Ru(1)	114.57(7)	C(10)-N(1)-C(9)	111.17(18)
C(10)-N(1)-C(12)	120.26(18)	C(9)-N(1)-C(12)	128.34(19)
C(9)-N(2)-C(11)	111.96(18)	C(9)-N(2)-C(18)	125.71(19)
C(11)-N(2)-C(18)	122.10(19)	O(1)-C(1)-Ru(1)	170.1(2)
C(7)-C(2)-C(3)	110.74(19)	C(7)-C(2)-Ru(1)	125.24(15)
C(3)-C(2)-Ru(1)	123.50(16)	F(1)-C(3)-C(4)	114.64(19)
F(1)-C(3)-C(2)	120.5(2)	C(4)-C(3)-C(2)	124.9(2)
F(2)-C(4)-C(3)	118.6(2)	F(2)-C(4)-C(5)	119.0(2)
C(3)-C(4)-C(5)	122.4(2)	C(4)-C(5)-C(6)	114.8(2)
C(4)-C(5)-C(8)	121.1(2)	C(6)-C(5)-C(8)	124.1(2)
F(3)-C(6)-C(7)	118.3(2)	F(3)-C(6)-C(5)	120.3(2)
C(7)-C(6)-C(5)	121.3(2)	F(4)-C(7)-C(6)	113.56(19)
F(4)-C(7)-C(2)	120.62(19)	C(6)-C(7)-C(2)	125.8(2)
F(7A)-C(8)-F(6A)	109.5(13)	F(7A)-C(8)-F(5)	116.2(13)
F(6A)-C(8)-F(5)	83.8(9)	F(7A)-C(8)-F(7)	15.3(16)
F(6A)-C(8)-F(7)	121.8(9)	F(5)-C(8)-F(7)	106.4(7)
F(7A)-C(8)-F(5A)	104.7(15)	F(6A)-C(8)-F(5A)	100.3(13)
F(5)-C(8)-F(5A)	17.6(14)	F(7)-C(8)-F(5A)	92.6(11)
F(7A)-C(8)-F(6)	89.3(12)	F(6A)-C(8)-F(6)	26.2(10)
F(5)-C(8)-F(6)	107.8(6)	F(7)-C(8)-F(6)	103.8(6)
F(5A)-C(8)-F(6)	122.7(11)	F(7A)-C(8)-C(5)	114.6(11)
F(6A)-C(8)-C(5)	113.7(7)	F(5)-C(8)-C(5)	115.0(4)
F(7)-C(8)-C(5)	112.5(5)	F(5A)-C(8)-C(5)	112.7(9)

F(6)-C(8)-C(5)	110.5(5)	N(2)-C(9)-N(1)	102.25(18)
N(2)-C(9)-Ru(1)	129.01(15)	N(1)-C(9)-Ru(1)	128.48(15)
C(11)-C(10)-N(1)	107.7(2)	C(11)-C(10)-H(10)	126.1
N(1)-C(10)-H(10)	126.1	C(10)-C(11)-N(2)	106.9(2)
C(10)-C(11)-H(11)	126.5	N(2)-C(11)-H(11)	126.5
N(1)-C(12)-C(17)	111.1(2)	N(1)-C(12)-C(13)	109.19(18)
C(17)-C(12)-C(13)	109.98(19)	C(14)-C(13)-C(12)	110.7(2)
C(14)-C(13)-H(13A)	109.5	C(12)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5	C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	108.1	C(15)-C(14)-C(13)	111.0(2)
C(15)-C(14)-H(14A)	109.4	C(13)-C(14)-H(14A)	109.4
C(15)-C(14)-H(14B)	109.4	C(13)-C(14)-H(14B)	109.4
H(14A)-C(14)-H(14B)	108.0	C(16)-C(15)-C(14)	110.9(2)
C(16)-C(15)-H(15A)	109.5	C(14)-C(15)-H(15A)	109.5
C(16)-C(15)-H(15B)	109.5	C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	108.1	C(15)-C(16)-C(17)	111.9(2)
C(15)-C(16)-H(16A)	109.2	C(17)-C(16)-H(16A)	109.2
C(15)-C(16)-H(16B)	109.2	C(17)-C(16)-H(16B)	109.2
H(16A)-C(16)-H(16B)	107.9	C(12)-C(17)-C(16)	110.2(2)
C(12)-C(17)-H(17A)	109.6	C(16)-C(17)-H(17A)	109.6
C(12)-C(17)-H(17B)	109.6	C(16)-C(17)-H(17B)	109.6
H(17A)-C(17)-H(17B)	108.1	N(2)-C(18)-C(19)	110.00(19)
N(2)-C(18)-C(23)	111.65(19)	C(19)-C(18)-C(23)	110.82(19)
C(18)-C(19)-C(20)	110.5(2)	C(18)-C(19)-H(19A)	109.6
C(20)-C(19)-H(19A)	109.6	C(18)-C(19)-H(19B)	109.6
C(20)-C(19)-H(19B)	109.6	H(19A)-C(19)-H(19B)	108.1
C(21)-C(20)-C(19)	110.9(2)	C(21)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20A)	109.5	C(21)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20B)	109.5	H(20A)-C(20)-H(20B)	108.0
C(20)-C(21)-C(22)	110.8(2)	C(20)-C(21)-H(21A)	109.5
C(22)-C(21)-H(21A)	109.5	C(20)-C(21)-H(21B)	109.5
C(22)-C(21)-H(21B)	109.5	H(21A)-C(21)-H(21B)	108.1
C(23)-C(22)-C(21)	111.2(2)	C(23)-C(22)-H(22A)	109.4
C(21)-C(22)-H(22A)	109.4	C(23)-C(22)-H(22B)	109.4
C(21)-C(22)-H(22B)	109.4	H(22A)-C(22)-H(22B)	108.0
C(22)-C(23)-C(18)	109.9(2)	C(22)-C(23)-H(23A)	109.7
C(18)-C(23)-H(23A)	109.7	C(22)-C(23)-H(23B)	109.7
C(18)-C(23)-H(23B)	109.7	H(23A)-C(23)-H(23B)	108.2
C(25)-C(24)-P(1)	113.80(15)	C(25)-C(24)-H(24B)	108.8
P(1)-C(24)-H(24B)	108.8	C(25)-C(24)-H(24A)	108.8
P(1)-C(24)-H(24A)	108.8	H(24B)-C(24)-H(24A)	107.7
C(26)-C(25)-C(24)	113.48(19)	C(26)-C(25)-H(25A)	108.9
C(24)-C(25)-H(25A)	108.9	C(26)-C(25)-H(25B)	108.9
C(24)-C(25)-H(25B)	108.9	H(25A)-C(25)-H(25B)	107.7
C(25)-C(26)-P(2)	113.85(15)	C(25)-C(26)-H(26A)	108.8
P(2)-C(26)-H(26A)	108.8	C(25)-C(26)-H(26B)	108.8
P(2)-C(26)-H(26B)	108.8	H(26A)-C(26)-H(26B)	107.7
C(32)-C(27)-C(28)	118.3(2)	C(32)-C(27)-P(1)	120.72(17)
C(28)-C(27)-P(1)	120.86(17)	C(29)-C(28)-C(27)	120.9(2)
C(29)-C(28)-H(28)	119.6	C(27)-C(28)-H(28)	119.6
C(30)-C(29)-C(28)	120.2(2)	C(30)-C(29)-H(29)	119.9
C(28)-C(29)-H(29)	119.9	C(29)-C(30)-C(31)	119.9(2)
C(29)-C(30)-H(30)	120.1	C(31)-C(30)-H(30)	120.1
C(30)-C(31)-C(32)	119.9(2)	C(30)-C(31)-H(31)	120.0
C(32)-C(31)-H(31)	120.0	C(27)-C(32)-C(31)	120.8(2)

C(27)-C(32)-H(32)	119.6	C(31)-C(32)-H(32)	119.6
C(38)-C(33)-C(34)	118.4(2)	C(38)-C(33)-P(1)	119.79(17)
C(34)-C(33)-P(1)	121.68(16)	C(35)-C(34)-C(33)	120.5(2)
C(35)-C(34)-H(34)	119.8	C(33)-C(34)-H(34)	119.8
C(36)-C(35)-C(34)	120.5(2)	C(36)-C(35)-H(35)	119.8
C(34)-C(35)-H(35)	119.8	C(37)-C(36)-C(35)	119.5(2)
C(37)-C(36)-H(36)	120.3	C(35)-C(36)-H(36)	120.3
C(36)-C(37)-C(38)	120.3(2)	C(36)-C(37)-H(37)	119.8
C(38)-C(37)-H(37)	119.8	C(37)-C(38)-C(33)	120.8(2)
C(37)-C(38)-H(38)	119.6	C(33)-C(38)-H(38)	119.6
C(44)-C(39)-C(40)	118.8(2)	C(44)-C(39)-P(2)	120.29(17)
C(40)-C(39)-P(2)	120.61(18)	C(41)-C(40)-C(39)	119.9(3)
C(41)-C(40)-H(40)	120.1	C(39)-C(40)-H(40)	120.1
C(42)-C(41)-C(40)	120.7(3)	C(42)-C(41)-H(41)	119.7
C(40)-C(41)-H(41)	119.7	C(43)-C(42)-C(41)	120.2(2)
C(43)-C(42)-H(42)	119.9	C(41)-C(42)-H(42)	119.9
C(42)-C(43)-C(44)	120.0(3)	C(42)-C(43)-H(43)	120.0
C(44)-C(43)-H(43)	120.0	C(39)-C(44)-C(43)	120.4(2)
C(39)-C(44)-H(44)	119.8	C(43)-C(44)-H(44)	119.8
C(50)-C(45)-C(46)	118.4(2)	C(50)-C(45)-P(2)	120.78(19)
C(46)-C(45)-P(2)	120.79(18)	C(45)-C(46)-C(47)	120.8(3)
C(45)-C(46)-H(46)	119.6	C(47)-C(46)-H(46)	119.6
C(48)-C(47)-C(46)	119.9(3)	C(48)-C(47)-H(47)	120.0
C(46)-C(47)-H(47)	120.0	C(49)-C(48)-C(47)	119.8(3)
C(49)-C(48)-H(48)	120.1	C(47)-C(48)-H(48)	120.1
C(48)-C(49)-C(50)	120.4(3)	C(48)-C(49)-H(49)	119.8
C(50)-C(49)-H(49)	119.8	C(45)-C(50)-C(49)	120.6(3)
C(45)-C(50)-H(50)	119.7	C(49)-C(50)-H(50)	119.7
C(52)-C(51)-C(56)	119.4(4)	C(52)-C(51)-H(51)	120.3
C(56)-C(51)-H(51)	120.3	C(53)-C(52)-C(51)	120.8(4)
C(53)-C(52)-H(52)	119.6	C(51)-C(52)-H(52)	119.6
C(54)-C(53)-C(52)	120.3(4)	C(54)-C(53)-H(53)	119.9
C(52)-C(53)-H(53)	119.9	C(53)-C(54)-C(55)	120.1(4)
C(53)-C(54)-H(54)	119.9	C(55)-C(54)-H(54)	119.9
C(56)-C(55)-C(54)	119.7(4)	C(56)-C(55)-H(55)	120.1
C(54)-C(55)-H(55)	120.1	C(55)-C(56)-C(51)	119.6(4)
C(55)-C(56)-H(56)	120.2	C(51)-C(56)-H(56)	120.2

Table 132. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(ICy)(dppp)(CO)($C_6F_4CF_3$)H **(81)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	18(1)	17(1)	20(1)	-8(1)	2(1)	-3(1)
P(1)	19(1)	17(1)	21(1)	-8(1)	1(1)	-4(1)
P(2)	22(1)	21(1)	22(1)	-10(1)	2(1)	-6(1)
F(1)	35(1)	26(1)	37(1)	-15(1)	-3(1)	3(1)
F(2)	55(1)	35(1)	54(1)	-31(1)	0(1)	0(1)
F(3)	41(1)	43(1)	31(1)	-16(1)	-8(1)	-2(1)
F(4)	40(1)	23(1)	31(1)	-10(1)	-5(1)	1(1)
F(5)	86(3)	69(4)	72(5)	-53(4)	-45(3)	26(3)
F(5A)	270(20)	93(9)	44(6)	-23(6)	-49(11)	-49(11)
F(6)	96(6)	63(2)	76(3)	-42(2)	-4(3)	-44(2)

F(6A)	97(11)	250(20)	121(14)	-149(15)	64(9)	-122(13)
F(7)	57(3)	106(5)	61(3)	-66(3)	8(3)	-8(3)
F(7A)	141(17)	143(15)	125(16)	-120(14)	-48(11)	71(12)
O(1)	31(1)	27(1)	35(1)	-8(1)	-1(1)	0(1)
N(1)	22(1)	21(1)	34(1)	-8(1)	5(1)	-4(1)
N(2)	22(1)	22(1)	28(1)	-8(1)	4(1)	-4(1)
C(1)	19(1)	30(1)	28(1)	-16(1)	7(1)	-11(1)
C(2)	18(1)	26(1)	19(1)	-11(1)	6(1)	-11(1)
C(3)	23(1)	28(1)	28(1)	-11(1)	4(1)	-4(1)
C(4)	35(1)	26(1)	38(1)	-20(1)	9(1)	-5(1)
C(5)	30(1)	36(1)	35(1)	-22(1)	4(1)	-9(1)
C(6)	28(1)	35(1)	23(1)	-11(1)	1(1)	-8(1)
C(7)	26(1)	23(1)	28(1)	-11(1)	4(1)	-6(1)
C(8)	48(2)	51(2)	49(2)	-35(2)	0(2)	-8(2)
C(9)	25(1)	21(1)	19(1)	-10(1)	4(1)	-7(1)
C(10)	29(1)	23(1)	44(2)	-6(1)	9(1)	-9(1)
C(11)	23(1)	30(1)	43(2)	-9(1)	7(1)	-9(1)
C(12)	28(1)	18(1)	31(1)	-6(1)	3(1)	2(1)
C(13)	36(1)	28(1)	34(1)	-11(1)	2(1)	0(1)
C(14)	41(2)	37(2)	38(2)	-10(1)	-4(1)	6(1)
C(15)	47(2)	26(1)	39(2)	-4(1)	6(1)	7(1)
C(16)	47(2)	29(1)	42(2)	-13(1)	9(1)	4(1)
C(17)	40(2)	29(1)	33(1)	-11(1)	5(1)	-3(1)
C(18)	21(1)	23(1)	34(1)	-9(1)	1(1)	1(1)
C(19)	32(1)	36(1)	46(2)	-20(1)	-9(1)	2(1)
C(20)	44(2)	35(2)	62(2)	-27(1)	-3(1)	2(1)
C(21)	33(1)	33(1)	37(2)	-9(1)	6(1)	5(1)
C(22)	33(2)	46(2)	35(2)	-13(1)	-4(1)	6(1)
C(23)	31(1)	37(1)	32(1)	-17(1)	-4(1)	2(1)
C(24)	22(1)	23(1)	24(1)	-7(1)	3(1)	-6(1)
C(25)	27(1)	28(1)	22(1)	-9(1)	4(1)	-7(1)
C(26)	29(1)	29(1)	21(1)	-11(1)	1(1)	-6(1)
C(27)	20(1)	20(1)	28(1)	-13(1)	1(1)	-4(1)
C(28)	27(1)	28(1)	29(1)	-12(1)	2(1)	-5(1)
C(29)	23(1)	41(1)	41(2)	-22(1)	7(1)	-5(1)
C(30)	22(1)	35(1)	50(2)	-26(1)	-4(1)	3(1)
C(31)	29(1)	28(1)	43(2)	-12(1)	-8(1)	1(1)
C(32)	22(1)	26(1)	32(1)	-10(1)	0(1)	-3(1)
C(33)	21(1)	19(1)	26(1)	-10(1)	8(1)	-7(1)
C(34)	32(1)	23(1)	29(1)	-10(1)	0(1)	-6(1)
C(35)	38(2)	33(1)	34(1)	-17(1)	-4(1)	-8(1)
C(36)	45(2)	30(1)	35(1)	-21(1)	10(1)	-13(1)
C(37)	37(1)	21(1)	46(2)	-16(1)	6(1)	-3(1)
C(38)	26(1)	24(1)	33(1)	-11(1)	1(1)	-5(1)
C(39)	29(1)	24(1)	29(1)	-13(1)	9(1)	-9(1)
C(40)	37(2)	38(1)	41(2)	-25(1)	10(1)	-13(1)
C(41)	58(2)	41(2)	52(2)	-33(1)	20(2)	-20(1)
C(42)	52(2)	27(1)	59(2)	-23(1)	30(2)	-11(1)
C(43)	36(2)	27(1)	43(2)	-9(1)	11(1)	0(1)
C(44)	31(1)	24(1)	31(1)	-12(1)	9(1)	-6(1)
C(45)	23(1)	37(1)	29(1)	-22(1)	6(1)	-10(1)
C(46)	28(1)	38(1)	44(2)	-22(1)	0(1)	-5(1)
C(47)	25(1)	57(2)	56(2)	-34(2)	-2(1)	0(1)
C(48)	23(1)	75(2)	71(2)	-55(2)	6(1)	-11(1)
C(49)	36(2)	48(2)	76(2)	-36(2)	14(2)	-22(1)

C(50)	32(1)	37(1)	46(2)	-20(1)	4(1)	-14(1)
C(51)	64(2)	69(2)	89(3)	-29(2)	-20(2)	-11(2)
C(52)	62(2)	73(2)	66(2)	-22(2)	9(2)	-26(2)
C(53)	65(2)	54(2)	57(2)	-3(2)	19(2)	-8(2)
C(54)	68(2)	73(2)	56(2)	-4(2)	2(2)	-2(2)
C(55)	90(3)	70(2)	70(3)	-37(2)	8(2)	-11(2)
C(56)	63(3)	63(2)	120(4)	-47(3)	3(2)	1(2)

Table 133. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(ICy)(dppp)(CO)($C_6F_4CF_3$)H **(81)**.

Atom	x	y	z	U(eq)
H(10)	9508	5861	5807	41
H(11)	10841	4282	6394	40
H(13A)	8029	6357	4754	40
H(13B)	7486	5341	4852	40
H(14A)	6436	7042	3975	50
H(14B)	5919	6295	4958	50
H(15A)	6926	8117	4711	51
H(15B)	5748	8099	4831	51
H(16A)	5985	6773	6451	49
H(16B)	6541	7789	6326	49
H(17A)	8100	6808	6230	42
H(17B)	7580	6079	7221	42
H(19A)	10642	2243	6056	45
H(19B)	9616	1762	6439	45
H(20A)	10493	88	7591	54
H(20B)	10919	320	6527	54
H(21A)	12310	966	6862	45
H(21B)	12239	-233	7721	45
H(22A)	11515	549	8756	49
H(22B)	12548	1014	8379	49
H(23A)	11685	2668	7198	40
H(23B)	11275	2468	8261	40
H(24B)	5683	612	10082	29
H(24A)	6869	358	10041	29
H(25A)	5936	2377	10065	31
H(25B)	6257	1308	11060	31
H(26A)	7962	1331	10472	31
H(26B)	7550	2298	10786	31
H(28)	4356	1563	9547	34
H(29)	2774	2590	9232	40
H(30)	2440	4204	7800	40
H(31)	3680	4764	6652	41
H(32)	5265	3723	6954	33
H(34)	4739	1446	7272	34
H(35)	4478	62	6818	41
H(36)	5502	-1635	7465	40
H(37)	6810	-1933	8552	41
H(38)	7095	-548	8991	34
H(40)	7710	4301	10235	43
H(41)	6620	5744	10333	53
H(42)	5243	6568	9270	53
H(43)	4936	5959	8098	45

H(44)	6018	4513	7979	34
H(46)	9515	1626	10196	42
H(47)	11089	1887	10564	52
H(48)	11535	3655	9925	57
H(49)	10452	5134	8839	59
H(50)	8872	4883	8477	44
H(51)	10331	1621	4472	90
H(52)	9028	2742	4749	81
H(53)	7821	3770	3553	80
H(54)	7859	3632	2086	90
H(55)	9173	2528	1769	89
H(56)	10436	1553	2946	96
H(1)	6836(13)	3613(11)	7252(14)	24(6)

Table 134. Dihedral angles [°] for Ru(ICy)(dppp)(CO)($C_6F_4CF_3$)H **(81)**.

Atom1 - Atom2 - Atom3 - Atom4	Dihedral
C(1) - Ru(1) - P(1) - C(24)	48.17(10)
C(9) - Ru(1) - P(1) - C(24)	-127.6(3)
C(2) - Ru(1) - P(1) - C(24)	145.22(10)
P(2) - Ru(1) - P(1) - C(24)	-38.85(8)
C(1) - Ru(1) - P(1) - C(33)	-68.56(10)
C(9) - Ru(1) - P(1) - C(33)	115.6(3)
C(2) - Ru(1) - P(1) - C(33)	28.50(10)
P(2) - Ru(1) - P(1) - C(33)	-155.58(8)
C(1) - Ru(1) - P(1) - C(27)	169.60(10)
C(9) - Ru(1) - P(1) - C(27)	-6.2(3)
C(2) - Ru(1) - P(1) - C(27)	-93.34(10)
P(2) - Ru(1) - P(1) - C(27)	82.58(8)
C(1) - Ru(1) - P(2) - C(39)	-169.06(11)
C(9) - Ru(1) - P(2) - C(39)	88.19(11)
C(2) - Ru(1) - P(2) - C(39)	-3.9(8)
P(1) - Ru(1) - P(2) - C(39)	-80.21(9)
C(1) - Ru(1) - P(2) - C(45)	65.46(11)
C(9) - Ru(1) - P(2) - C(45)	-37.29(10)
C(2) - Ru(1) - P(2) - C(45)	-129.4(8)
P(1) - Ru(1) - P(2) - C(45)	154.31(9)
C(1) - Ru(1) - P(2) - C(26)	-50.61(11)
C(9) - Ru(1) - P(2) - C(26)	-153.36(10)
C(2) - Ru(1) - P(2) - C(26)	114.5(8)
P(1) - Ru(1) - P(2) - C(26)	38.24(8)
C(9) - Ru(1) - C(1) - O(1)	139.6(11)
C(2) - Ru(1) - C(1) - O(1)	-127.1(11)
P(2) - Ru(1) - C(1) - O(1)	51.8(11)
P(1) - Ru(1) - C(1) - O(1)	-39.5(11)
C(1) - Ru(1) - C(2) - C(7)	176.12(19)
C(9) - Ru(1) - C(2) - C(7)	-80.92(19)
P(2) - Ru(1) - C(2) - C(7)	11.1(9)
P(1) - Ru(1) - C(2) - C(7)	87.49(18)
C(1) - Ru(1) - C(2) - C(3)	5.19(19)
C(9) - Ru(1) - C(2) - C(3)	108.15(19)
P(2) - Ru(1) - C(2) - C(3)	-159.9(7)
P(1) - Ru(1) - C(2) - C(3)	-83.44(18)
C(7) - C(2) - C(3) - F(1)	178.35(19)

Ru(1) - C(2) - C(3) - F(1)	-9.6(3)
C(7) - C(2) - C(3) - C(4)	-2.7(3)
Ru(1) - C(2) - C(3) - C(4)	169.42(19)
F(1) - C(3) - C(4) - F(2)	0.6(3)
C(2) - C(3) - C(4) - F(2)	-178.4(2)
F(1) - C(3) - C(4) - C(5)	-179.3(2)
C(2) - C(3) - C(4) - C(5)	1.6(4)
F(2) - C(4) - C(5) - C(6)	180.0(2)
C(3) - C(4) - C(5) - C(6)	-0.1(4)
F(2) - C(4) - C(5) - C(8)	0.7(4)
C(3) - C(4) - C(5) - C(8)	-179.4(2)
C(4) - C(5) - C(6) - F(3)	179.1(2)
C(8) - C(5) - C(6) - F(3)	-1.6(4)
C(4) - C(5) - C(6) - C(7)	-0.1(4)
C(8) - C(5) - C(6) - C(7)	179.2(2)
F(3) - C(6) - C(7) - F(4)	0.1(3)
C(5) - C(6) - C(7) - F(4)	179.4(2)
F(3) - C(6) - C(7) - C(2)	179.5(2)
C(5) - C(6) - C(7) - C(2)	-1.3(4)
C(3) - C(2) - C(7) - F(4)	-178.19(19)
Ru(1) - C(2) - C(7) - F(4)	9.9(3)
C(3) - C(2) - C(7) - C(6)	2.5(3)
Ru(1) - C(2) - C(7) - C(6)	-169.42(19)
C(4) - C(5) - C(8) - F(7A)	-36.4(14)
C(6) - C(5) - C(8) - F(7A)	144.3(13)
C(4) - C(5) - C(8) - F(6A)	90.7(10)
C(6) - C(5) - C(8) - F(6A)	-88.6(10)
C(4) - C(5) - C(8) - F(5)	-175.0(6)
C(6) - C(5) - C(8) - F(5)	5.7(7)
C(4) - C(5) - C(8) - F(7)	-52.9(7)
C(6) - C(5) - C(8) - F(7)	127.8(6)
C(4) - C(5) - C(8) - F(5A)	-156.0(12)
C(6) - C(5) - C(8) - F(5A)	24.7(12)
C(4) - C(5) - C(8) - F(6)	62.6(5)
C(6) - C(5) - C(8) - F(6)	-116.7(4)
C(11) - N(2) - C(9) - N(1)	0.4(2)
C(18) - N(2) - C(9) - N(1)	-174.0(2)
C(11) - N(2) - C(9) - Ru(1)	-173.97(16)
C(18) - N(2) - C(9) - Ru(1)	11.6(3)
C(10) - N(1) - C(9) - N(2)	-0.6(2)
C(12) - N(1) - C(9) - N(2)	173.9(2)
C(10) - N(1) - C(9) - Ru(1)	173.85(17)
C(12) - N(1) - C(9) - Ru(1)	-11.7(3)
C(1) - Ru(1) - C(9) - N(2)	6.5(2)
C(2) - Ru(1) - C(9) - N(2)	-91.07(19)
P(2) - Ru(1) - C(9) - N(2)	93.12(18)
P(1) - Ru(1) - C(9) - N(2)	-177.80(17)
C(1) - Ru(1) - C(9) - N(1)	-166.52(19)
C(2) - Ru(1) - C(9) - N(1)	95.91(19)
P(2) - Ru(1) - C(9) - N(1)	-79.89(19)
P(1) - Ru(1) - C(9) - N(1)	9.2(4)
C(9) - N(1) - C(10) - C(11)	0.6(3)
C(12) - N(1) - C(10) - C(11)	-174.4(2)
N(1) - C(10) - C(11) - N(2)	-0.3(3)
C(9) - N(2) - C(11) - C(10)	-0.1(3)

C(18) - N(2) - C(11) - C(10)	174.6(2)
C(10) - N(1) - C(12) - C(17)	-60.1(3)
C(9) - N(1) - C(12) - C(17)	125.8(2)
C(10) - N(1) - C(12) - C(13)	61.4(3)
C(9) - N(1) - C(12) - C(13)	-112.7(2)
N(1) - C(12) - C(13) - C(14)	179.5(2)
C(17) - C(12) - C(13) - C(14)	-58.3(3)
C(12) - C(13) - C(14) - C(15)	57.1(3)
C(13) - C(14) - C(15) - C(16)	-55.2(3)
C(14) - C(15) - C(16) - C(17)	55.3(3)
N(1) - C(12) - C(17) - C(16)	178.45(19)
C(13) - C(12) - C(17) - C(16)	57.4(3)
C(15) - C(16) - C(17) - C(12)	-56.6(3)
C(9) - N(2) - C(18) - C(19)	86.0(3)
C(11) - N(2) - C(18) - C(19)	-87.9(3)
C(9) - N(2) - C(18) - C(23)	-150.5(2)
C(11) - N(2) - C(18) - C(23)	35.6(3)
N(2) - C(18) - C(19) - C(20)	-178.5(2)
C(23) - C(18) - C(19) - C(20)	57.6(3)
C(18) - C(19) - C(20) - C(21)	-56.0(3)
C(19) - C(20) - C(21) - C(22)	55.1(3)
C(20) - C(21) - C(22) - C(23)	-56.4(3)
C(21) - C(22) - C(23) - C(18)	57.6(3)
N(2) - C(18) - C(23) - C(22)	178.6(2)
C(19) - C(18) - C(23) - C(22)	-58.4(3)
C(33) - P(1) - C(24) - C(25)	-174.16(16)
C(27) - P(1) - C(24) - C(25)	-70.55(18)
Ru(1) - P(1) - C(24) - C(25)	59.98(17)
P(1) - C(24) - C(25) - C(26)	-75.2(2)
C(24) - C(25) - C(26) - P(2)	74.0(2)
C(39) - P(2) - C(26) - C(25)	72.24(18)
C(45) - P(2) - C(26) - C(25)	176.77(16)
Ru(1) - P(2) - C(26) - C(25)	-58.25(17)
C(24) - P(1) - C(27) - C(32)	156.88(18)
C(33) - P(1) - C(27) - C(32)	-99.67(19)
Ru(1) - P(1) - C(27) - C(32)	29.8(2)
C(24) - P(1) - C(27) - C(28)	-26.6(2)
C(33) - P(1) - C(27) - C(28)	76.82(19)
Ru(1) - P(1) - C(27) - C(28)	-153.67(15)
C(32) - C(27) - C(28) - C(29)	-0.5(3)
P(1) - C(27) - C(28) - C(29)	-177.09(18)
C(27) - C(28) - C(29) - C(30)	-0.5(4)
C(28) - C(29) - C(30) - C(31)	1.1(4)
C(29) - C(30) - C(31) - C(32)	-0.7(4)
C(28) - C(27) - C(32) - C(31)	1.0(3)
P(1) - C(27) - C(32) - C(31)	177.56(18)
C(30) - C(31) - C(32) - C(27)	-0.4(4)
C(24) - P(1) - C(33) - C(38)	-53.0(2)
C(27) - P(1) - C(33) - C(38)	-157.96(19)
Ru(1) - P(1) - C(33) - C(38)	70.8(2)
C(24) - P(1) - C(33) - C(34)	130.91(19)
C(27) - P(1) - C(33) - C(34)	26.0(2)
Ru(1) - P(1) - C(33) - C(34)	-105.20(18)
C(38) - C(33) - C(34) - C(35)	0.4(3)
P(1) - C(33) - C(34) - C(35)	176.50(19)

C(33) - C(34) - C(35) - C(36)	0.4(4)
C(34) - C(35) - C(36) - C(37)	-0.6(4)
C(35) - C(36) - C(37) - C(38)	0.0(4)
C(36) - C(37) - C(38) - C(33)	0.8(4)
C(34) - C(33) - C(38) - C(37)	-1.0(3)
P(1) - C(33) - C(38) - C(37)	-177.14(19)
C(45) - P(2) - C(39) - C(44)	144.76(19)
C(26) - P(2) - C(39) - C(44)	-112.7(2)
Ru(1) - P(2) - C(39) - C(44)	13.3(2)
C(45) - P(2) - C(39) - C(40)	-41.1(2)
C(26) - P(2) - C(39) - C(40)	61.4(2)
Ru(1) - P(2) - C(39) - C(40)	-172.63(16)
C(44) - C(39) - C(40) - C(41)	0.0(4)
P(2) - C(39) - C(40) - C(41)	-174.2(2)
C(39) - C(40) - C(41) - C(42)	0.0(4)
C(40) - C(41) - C(42) - C(43)	0.0(4)
C(41) - C(42) - C(43) - C(44)	-0.1(4)
C(40) - C(39) - C(44) - C(43)	0.0(3)
P(2) - C(39) - C(44) - C(43)	174.20(18)
C(42) - C(43) - C(44) - C(39)	0.1(4)
C(39) - P(2) - C(45) - C(50)	-39.9(2)
C(26) - P(2) - C(45) - C(50)	-141.5(2)
Ru(1) - P(2) - C(45) - C(50)	94.6(2)
C(39) - P(2) - C(45) - C(46)	141.0(2)
C(26) - P(2) - C(45) - C(46)	39.4(2)
Ru(1) - P(2) - C(45) - C(46)	-84.5(2)
C(50) - C(45) - C(46) - C(47)	3.1(4)
P(2) - C(45) - C(46) - C(47)	-177.8(2)
C(45) - C(46) - C(47) - C(48)	-0.5(4)
C(46) - C(47) - C(48) - C(49)	-2.4(4)
C(47) - C(48) - C(49) - C(50)	2.6(4)
C(46) - C(45) - C(50) - C(49)	-2.8(4)
P(2) - C(45) - C(50) - C(49)	178.1(2)
C(48) - C(49) - C(50) - C(45)	0.0(4)
C(56) - C(51) - C(52) - C(53)	0.5(6)
C(51) - C(52) - C(53) - C(54)	1.5(6)
C(52) - C(53) - C(54) - C(55)	-2.0(6)
C(53) - C(54) - C(55) - C(56)	0.3(6)
C(54) - C(55) - C(56) - C(51)	1.7(6)
C(52) - C(51) - C(56) - C(55)	-2.2(6)

Table 135. Crystal data and structure refinement for Ru(ICy)(dppp)(C_5F_4N)H **(82)**.

Compound	Ru(ICy)(dppp)(C_5F_4N)H **(82)**
Empirical formula	C60 H63 F4 N3 O P2 Ru
Formula weight	1081.14
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.2020(2)Å α = 69.866(1)°
	b = 13.9180(2)Å β = 73.345(1)°
	c = 18.9190(3)Å γ = 75.351(1)°
Volume	2613.92(7) $Å^3$
Z	2
Density (calculated)	1.374 Mg/m^3
Absorption coefficient	0.420 mm^{-1}
F(000)	1124
Crystal size	0.25 x 0.20 x 0.10 mm
Theta range for data collection	3.77 to 27.46°
Index ranges	-14<=h<=14; -18<=k<=18; -24<=l<=24
Reflections collected	38269
Independent reflections	11866 [R(int) = 0.0758]
Reflections observed (>2σ)	9273
Data Completeness	0.993
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.96 and 0.83
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11866 / 1 / 683
Goodness-of-fit on F^2	1.013
Final R indices [I>2σ(I)]	R1 = 0.0387 wR2 = 0.0875
R indices (all data)	R1 = 0.0604 wR2 = 0.0970
Largest diff. peak and hole	0.392 and -0.880 $eÅ^{-3}$

Table 136. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for Ru(ICy)(dppp)(C_5F_4N)H **(82)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	2128(1)	1496(1)	7245(1)	18(1)
P(1)	3760(1)	928(1)	6327(1)	20(1)
P(2)	1581(1)	3106(1)	6377(1)	20(1)
F(1)	4179(1)	460(1)	8451(1)	36(1)
F(2)	4537(1)	-1370(1)	9472(1)	42(1)
F(3)	1686(2)	-2557(1)	8867(1)	42(1)
F(4)	1098(1)	-781(1)	7853(1)	31(1)
O(1)	248(2)	982(1)	6592(1)	35(1)
N(1)	1254(2)	2642(1)	8544(1)	23(1)
N(2)	-121(2)	1718(1)	8671(1)	24(1)
N(3)	3126(2)	-1973(2)	9172(1)	31(1)
C(1)	911(2)	1119(2)	6905(1)	23(1)
C(2)	1006(2)	1993(2)	8212(1)	20(1)
C(3)	297(2)	2751(2)	9180(1)	29(1)
C(4)	-555(2)	2188(2)	9255(1)	30(1)
C(5)	2338(2)	3190(2)	8300(1)	26(1)

C(6)	1909(3)	4340(2)	8238(2)	36(1)
C(7)	3032(3)	4910(2)	7979(2)	44(1)
C(8)	3960(3)	4398(2)	8511(2)	44(1)
C(9)	4373(3)	3246(2)	8578(2)	49(1)
C(10)	3235(2)	2698(2)	8847(2)	35(1)
C(11)	-821(2)	999(2)	8603(1)	24(1)
C(12)	-960(2)	80(2)	9332(1)	31(1)
C(13)	-1676(3)	-665(2)	9261(2)	40(1)
C(14)	-2971(3)	-120(2)	9099(2)	43(1)
C(15)	-2826(3)	805(2)	8369(2)	41(1)
C(16)	-2112(2)	1562(2)	8429(2)	34(1)
C(17)	2579(2)	21(2)	8066(1)	19(1)
C(18)	3465(2)	-228(2)	8514(1)	25(1)
C(19)	3689(2)	-1189(2)	9044(1)	29(1)
C(20)	2290(2)	-1770(2)	8750(1)	29(1)
C(21)	2004(2)	-835(2)	8222(1)	25(1)
C(22)	3426(2)	1376(2)	5356(1)	25(1)
C(23)	3161(2)	2564(2)	5038(1)	26(1)
C(24)	1824(2)	3055(2)	5381(1)	24(1)
C(25)	5351(2)	1235(2)	6112(1)	22(1)
C(26)	6234(2)	1069(2)	5452(1)	28(1)
C(27)	7442(2)	1281(2)	5281(2)	33(1)
C(28)	7802(2)	1660(2)	5759(2)	34(1)
C(29)	6957(2)	1813(2)	6416(2)	32(1)
C(30)	5732(2)	1602(2)	6595(1)	27(1)
C(31)	4125(2)	-489(2)	6523(1)	23(1)
C(32)	5188(2)	-1081(2)	6806(1)	31(1)
C(33)	5370(3)	-2159(2)	7024(2)	39(1)
C(34)	4509(3)	-2657(2)	6962(2)	40(1)
C(35)	3449(3)	-2085(2)	6685(2)	36(1)
C(36)	3256(2)	-1012(2)	6470(1)	29(1)
C(37)	2337(2)	4221(2)	6179(1)	23(1)
C(38)	1689(2)	5240(2)	6006(1)	30(1)
C(39)	2318(3)	6069(2)	5804(2)	36(1)
C(40)	3605(3)	5895(2)	5747(2)	35(1)
C(41)	4260(2)	4891(2)	5917(2)	34(1)
C(42)	3636(2)	4056(2)	6142(1)	27(1)
C(43)	-115(2)	3688(2)	6561(1)	23(1)
C(44)	-653(2)	3985(2)	7232(1)	29(1)
C(45)	-1928(2)	4421(2)	7397(2)	35(1)
C(46)	-2679(2)	4563(2)	6890(2)	40(1)
C(47)	-2157(2)	4282(2)	6222(2)	40(1)
C(48)	-886(2)	3847(2)	6058(2)	32(1)
C(49)	1818(19)	3680(20)	10751(12)	104(5)
C(50)	1599(16)	4674(12)	10493(11)	71(4)
C(51)	2469(16)	5267(15)	10436(10)	60(4)
C(52)	3527(11)	4728(11)	10683(7)	53(3)
C(53)	3683(12)	3660(9)	10947(6)	67(3)
C(54)	2722(18)	3198(9)	10953(7)	96(5)
C(55)	-162(3)	-1502(3)	6827(2)	53(1)
C(56)	-116(3)	-2512(3)	7286(2)	56(1)
C(57)	-597(3)	-3194(2)	7106(2)	55(1)
C(58)	-1099(3)	-2870(2)	6470(2)	52(1)
C(59)	-1134(3)	-1878(3)	6020(2)	58(1)
C(60)	-663(3)	-1181(2)	6189(2)	55(1)

C(49A)	3878(11)	4116(16)	10882(8)	89(8)
C(50A)	3374(15)	3215(10)	11102(7)	66(5)
C(51A)	2218(14)	3257(12)	10947(5)	240(40)
C(52A)	1567(10)	4201(16)	10571(9)	170(30)
C(53A)	2070(20)	5103(10)	10351(8)	99(17)
C(54A)	3230(20)	5060(11)	10506(6)	126(18)

Table 137. Bond lengths [Å] and angles [°] for Ru(ICy)(dppp)(C_5F_4N)H **(82)**.

Ru(1)-C(1)	1.909(2)	Ru(1)-C(2)	2.127(2)
Ru(1)-C(17)	2.149(2)	Ru(1)-P(1)	2.3197(6)
Ru(1)-P(2)	2.3326(6)	Ru(1)-H(1)	1.6013
P(1)-C(31)	1.835(2)	P(1)-C(25)	1.837(2)
P(1)-C(22)	1.842(2)	P(2)-C(37)	1.830(2)
P(2)-C(24)	1.848(2)	P(2)-C(43)	1.851(2)
F(1)-C(18)	1.352(3)	F(2)-C(19)	1.341(3)
F(3)-C(20)	1.352(3)	F(4)-C(21)	1.361(3)
O(1)-C(1)	1.158(3)	N(1)-C(2)	1.380(3)
N(1)-C(3)	1.387(3)	N(1)-C(5)	1.474(3)
N(2)-C(2)	1.372(3)	N(2)-C(4)	1.383(3)
N(2)-C(11)	1.475(3)	N(3)-C(19)	1.315(3)
N(3)-C(20)	1.316(3)	C(3)-C(4)	1.330(3)
C(3)-H(3)	0.9500	C(4)-H(4)	0.9500
C(5)-C(10)	1.520(4)	C(5)-C(6)	1.523(3)
C(5)-H(5)	1.0000	C(6)-C(7)	1.528(4)
C(6)-H(6A)	0.9900	C(6)-H(6B)	0.9900
C(7)-C(8)	1.527(4)	C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900	C(8)-C(9)	1.523(4)
C(8)-H(8A)	0.9900	C(8)-H(8B)	0.9900
C(9)-C(10)	1.522(4)	C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900	C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900	C(11)-C(12)	1.525(3)
C(11)-C(16)	1.529(3)	C(11)-H(11)	1.0000
C(12)-C(13)	1.521(4)	C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900	C(13)-C(14)	1.520(4)
C(13)-H(13A)	0.9900	C(13)-H(13B)	0.9900
C(14)-C(15)	1.531(4)	C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900	C(15)-C(16)	1.525(4)
C(15)-H(15A)	0.9900	C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9900	C(16)-H(16B)	0.9900
C(17)-C(18)	1.388(3)	C(17)-C(21)	1.399(3)
C(18)-C(19)	1.381(3)	C(20)-C(21)	1.368(3)
C(22)-C(23)	1.534(3)	C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900	C(23)-C(24)	1.536(3)
C(23)-H(23A)	0.9900	C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9900	C(24)-H(24B)	0.9900
C(25)-C(30)	1.390(3)	C(25)-C(26)	1.402(3)
C(26)-C(27)	1.380(3)	C(26)-H(26)	0.9500
C(27)-C(28)	1.380(4)	C(27)-H(27)	0.9500
C(28)-C(29)	1.377(4)	C(28)-H(28)	0.9500
C(29)-C(30)	1.397(3)	C(29)-H(29)	0.9500
C(30)-H(30)	0.9500	C(31)-C(32)	1.396(3)
C(31)-C(36)	1.397(3)	C(32)-C(33)	1.390(3)
C(32)-H(32)	0.9500	C(33)-C(34)	1.374(4)
C(33)-H(33)	0.9500	C(34)-C(35)	1.382(4)

C(34)-H(34)	0.9500	C(35)-C(36)	1.383(3)
C(35)-H(35)	0.9500	C(36)-H(36)	0.9500
C(37)-C(38)	1.394(3)	C(37)-C(42)	1.400(3)
C(38)-C(39)	1.388(3)	C(38)-H(38)	0.9500
C(39)-C(40)	1.379(4)	C(39)-H(39)	0.9500
C(40)-C(41)	1.379(4)	C(40)-H(40)	0.9500
C(41)-C(42)	1.386(3)	C(41)-H(41)	0.9500
C(42)-H(42)	0.9500	C(43)-C(48)	1.389(3)
C(43)-C(44)	1.394(3)	C(44)-C(45)	1.393(3)
C(44)-H(44)	0.9500	C(45)-C(46)	1.384(4)
C(45)-H(45)	0.9500	C(46)-C(47)	1.376(4)
C(46)-H(46)	0.9500	C(47)-C(48)	1.389(3)
C(47)-H(47)	0.9500	C(48)-H(48)	0.9500
C(49)-C(50)	1.28(4)	C(49)-C(54)	1.15(3)
C(49)-H(49)	0.9500	C(50)-C(51)	1.39(2)
C(50)-H(50)	0.9500	C(51)-C(52)	1.35(2)
C(51)-H(51)	0.9500	C(52)-C(53)	1.377(16)
C(52)-H(52)	0.9500	C(53)-C(54)	1.38(2)
C(53)-H(53)	0.9500	C(54)-H(54)	0.9500
C(55)-C(60)	1.365(5)	C(55)-C(56)	1.372(5)
C(55)-H(55)	0.9500	C(56)-C(57)	1.376(4)
C(56)-H(56)	0.9500	C(57)-C(58)	1.362(5)
C(57)-H(57)	0.9500	C(58)-C(59)	1.348(5)
C(58)-H(58)	0.9500	C(59)-C(60)	1.375(4)
C(59)-H(59)	0.9500	C(60)-H(60)	0.9500
C(49A)-C(50A)	1.3900	C(49A)-C(54A)	1.3900
C(49A)-H(49A)	0.9500	C(50A)-C(51A)	1.3900
C(50A)-H(50A)	0.9500	C(51A)-C(52A)	1.3900
C(51A)-H(51A)	0.9500	C(52A)-C(53A)	1.3900
C(52A)-H(52A)	0.9500	C(53A)-C(54A)	1.3900
C(53A)-H(53A)	0.9500	C(54A)-H(54A)	0.9500
C(1)-Ru(1)-C(2)	102.31(9)	C(1)-Ru(1)-C(17)	96.94(9)
C(2)-Ru(1)-C(17)	86.10(8)	C(1)-Ru(1)-P(1)	91.29(7)
C(2)-Ru(1)-P(1)	165.75(6)	C(17)-Ru(1)-P(1)	88.08(5)
C(1)-Ru(1)-P(2)	82.53(7)	C(2)-Ru(1)-P(2)	92.48(6)
C(17)-Ru(1)-P(2)	178.34(6)	P(1)-Ru(1)-P(2)	93.49(2)
C(1)-Ru(1)-H(1)	172.8	C(2)-Ru(1)-H(1)	82.4
C(17)-Ru(1)-H(1)	88.8	P(1)-Ru(1)-H(1)	84.5
P(2)-Ru(1)-H(1)	91.8	C(31)-P(1)-C(25)	100.91(10)
C(31)-P(1)-C(22)	102.68(10)	C(25)-P(1)-C(22)	101.33(11)
C(31)-P(1)-Ru(1)	114.11(7)	C(25)-P(1)-Ru(1)	121.43(7)
C(22)-P(1)-Ru(1)	113.84(7)	C(37)-P(2)-C(24)	99.65(10)
C(37)-P(2)-C(43)	101.64(10)	C(24)-P(2)-C(43)	100.47(11)
C(37)-P(2)-Ru(1)	122.82(8)	C(24)-P(2)-Ru(1)	113.56(7)
C(43)-P(2)-Ru(1)	115.36(7)	C(2)-N(1)-C(3)	110.53(18)
C(2)-N(1)-C(5)	128.61(17)	C(3)-N(1)-C(5)	120.85(18)
C(2)-N(2)-C(4)	111.32(19)	C(2)-N(2)-C(11)	127.31(18)
C(4)-N(2)-C(11)	121.35(18)	C(19)-N(3)-C(20)	114.1(2)
O(1)-C(1)-Ru(1)	169.8(2)	N(2)-C(2)-N(1)	103.36(17)
N(2)-C(2)-Ru(1)	128.16(15)	N(1)-C(2)-Ru(1)	128.45(15)
C(4)-C(3)-N(1)	107.7(2)	C(4)-C(3)-H(3)	126.2
N(1)-C(3)-H(3)	126.2	C(3)-C(4)-N(2)	107.1(2)
C(3)-C(4)-H(4)	126.4	N(2)-C(4)-H(4)	126.4
N(1)-C(5)-C(10)	111.26(19)	N(1)-C(5)-C(6)	111.65(19)

C(10)-C(5)-C(6)	109.9(2)	N(1)-C(5)-H(5)	108.0
C(10)-C(5)-H(5)	108.0	C(6)-C(5)-H(5)	108.0
C(5)-C(6)-C(7)	111.7(2)	C(5)-C(6)-H(6A)	109.3
C(7)-C(6)-H(6A)	109.3	C(5)-C(6)-H(6B)	109.3
C(7)-C(6)-H(6B)	109.3	H(6A)-C(6)-H(6B)	107.9
C(6)-C(7)-C(8)	111.2(2)	C(6)-C(7)-H(7A)	109.4
C(8)-C(7)-H(7A)	109.4	C(6)-C(7)-H(7B)	109.4
C(8)-C(7)-H(7B)	109.4	H(7A)-C(7)-H(7B)	108.0
C(9)-C(8)-C(7)	110.9(2)	C(9)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8A)	109.5	C(9)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8B)	109.5	H(8A)-C(8)-H(8B)	108.0
C(10)-C(9)-C(8)	111.0(2)	C(10)-C(9)-H(9A)	109.4
C(8)-C(9)-H(9A)	109.4	C(10)-C(9)-H(9B)	109.4
C(8)-C(9)-H(9B)	109.4	H(9A)-C(9)-H(9B)	108.0
C(9)-C(10)-C(5)	111.0(2)	C(9)-C(10)-H(10A)	109.4
C(5)-C(10)-H(10A)	109.4	C(9)-C(10)-H(10B)	109.4
C(5)-C(10)-H(10B)	109.4	H(10A)-C(10)-H(10B)	108.0
N(2)-C(11)-C(12)	110.72(19)	N(2)-C(11)-C(16)	111.04(18)
C(12)-C(11)-C(16)	110.99(19)	N(2)-C(11)-H(11)	108.0
C(12)-C(11)-H(11)	108.0	C(16)-C(11)-H(11)	108.0
C(13)-C(12)-C(11)	110.8(2)	C(13)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12A)	109.5	C(13)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12B)	109.5	H(12A)-C(12)-H(12B)	108.1
C(12)-C(13)-C(14)	111.5(2)	C(12)-C(13)-H(13A)	109.3
C(14)-C(13)-H(13A)	109.3	C(12)-C(13)-H(13B)	109.3
C(14)-C(13)-H(13B)	109.3	H(13A)-C(13)-H(13B)	108.0
C(13)-C(14)-C(15)	109.7(2)	C(13)-C(14)-H(14A)	109.7
C(15)-C(14)-H(14A)	109.7	C(13)-C(14)-H(14B)	109.7
C(15)-C(14)-H(14B)	109.7	H(14A)-C(14)-H(14B)	108.2
C(16)-C(15)-C(14)	111.9(2)	C(16)-C(15)-H(15A)	109.2
C(14)-C(15)-H(15A)	109.2	C(16)-C(15)-H(15B)	109.2
C(14)-C(15)-H(15B)	109.2	H(15A)-C(15)-H(15B)	107.9
C(15)-C(16)-C(11)	110.3(2)	C(15)-C(16)-H(16A)	109.6
C(11)-C(16)-H(16A)	109.6	C(15)-C(16)-H(16B)	109.6
C(11)-C(16)-H(16B)	109.6	H(16A)-C(16)-H(16B)	108.1
C(18)-C(17)-C(21)	110.3(2)	C(18)-C(17)-Ru(1)	125.92(16)
C(21)-C(17)-Ru(1)	123.77(16)	F(1)-C(18)-C(19)	115.4(2)
F(1)-C(18)-C(17)	121.7(2)	C(19)-C(18)-C(17)	122.9(2)
N(3)-C(19)-F(2)	115.4(2)	N(3)-C(19)-C(18)	124.7(2)
F(2)-C(19)-C(18)	119.9(2)	N(3)-C(20)-F(3)	115.9(2)
N(3)-C(20)-C(21)	124.5(2)	F(3)-C(20)-C(21)	119.6(2)
F(4)-C(21)-C(20)	115.3(2)	F(4)-C(21)-C(17)	121.3(2)
C(20)-C(21)-C(17)	123.4(2)	C(23)-C(22)-P(1)	112.69(16)
C(23)-C(22)-H(22A)	109.1	P(1)-C(22)-H(22A)	109.1
C(23)-C(22)-H(22B)	109.1	P(1)-C(22)-H(22B)	109.1
H(22A)-C(22)-H(22B)	107.8	C(22)-C(23)-C(24)	113.45(19)
C(22)-C(23)-H(23A)	108.9	C(24)-C(23)-H(23A)	108.9
C(22)-C(23)-H(23B)	108.9	C(24)-C(23)-H(23B)	108.9
H(23A)-C(23)-H(23B)	107.7	C(23)-C(24)-P(2)	115.07(16)
C(23)-C(24)-H(24A)	108.5	P(2)-C(24)-H(24A)	108.5
C(23)-C(24)-H(24B)	108.5	P(2)-C(24)-H(24B)	108.5
H(24A)-C(24)-H(24B)	107.5	C(30)-C(25)-C(26)	118.1(2)
C(30)-C(25)-P(1)	122.27(17)	C(26)-C(25)-P(1)	119.57(18)
C(27)-C(26)-C(25)	120.9(2)	C(27)-C(26)-H(26)	119.6
C(25)-C(26)-H(26)	119.6	C(28)-C(27)-C(26)	120.4(2)

C(28)-C(27)-H(27)	119.8	C(26)-C(27)-H(27)	119.8
C(29)-C(28)-C(27)	119.7(2)	C(29)-C(28)-H(28)	120.2
C(27)-C(28)-H(28)	120.2	C(28)-C(29)-C(30)	120.3(2)
C(28)-C(29)-H(29)	119.8	C(30)-C(29)-H(29)	119.8
C(25)-C(30)-C(29)	120.6(2)	C(25)-C(30)-H(30)	119.7
C(29)-C(30)-H(30)	119.7	C(32)-C(31)-C(36)	118.1(2)
C(32)-C(31)-P(1)	121.81(18)	C(36)-C(31)-P(1)	119.71(17)
C(33)-C(32)-C(31)	120.5(2)	C(33)-C(32)-H(32)	119.8
C(31)-C(32)-H(32)	119.8	C(34)-C(33)-C(32)	120.5(3)
C(34)-C(33)-H(33)	119.8	C(32)-C(33)-H(33)	119.8
C(33)-C(34)-C(35)	119.9(2)	C(33)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0	C(36)-C(35)-C(34)	120.1(3)
C(36)-C(35)-H(35)	120.0	C(34)-C(35)-H(35)	120.0
C(35)-C(36)-C(31)	121.0(2)	C(35)-C(36)-H(36)	119.5
C(31)-C(36)-H(36)	119.5	C(38)-C(37)-C(42)	118.3(2)
C(38)-C(37)-P(2)	122.51(18)	C(42)-C(37)-P(2)	119.06(17)
C(39)-C(38)-C(37)	120.8(2)	C(39)-C(38)-H(38)	119.6
C(37)-C(38)-H(38)	119.6	C(40)-C(39)-C(38)	120.2(2)
C(40)-C(39)-H(39)	119.9	C(38)-C(39)-H(39)	119.9
C(39)-C(40)-C(41)	119.7(2)	C(39)-C(40)-H(40)	120.1
C(41)-C(40)-H(40)	120.1	C(40)-C(41)-C(42)	120.5(2)
C(40)-C(41)-H(41)	119.7	C(42)-C(41)-H(41)	119.7
C(41)-C(42)-C(37)	120.4(2)	C(41)-C(42)-H(42)	119.8
C(37)-C(42)-H(42)	119.8	C(48)-C(43)-C(44)	118.0(2)
C(48)-C(43)-P(2)	122.97(17)	C(44)-C(43)-P(2)	119.04(18)
C(45)-C(44)-C(43)	121.0(2)	C(45)-C(44)-H(44)	119.5
C(43)-C(44)-H(44)	119.5	C(46)-C(45)-C(44)	119.9(2)
C(46)-C(45)-H(45)	120.0	C(44)-C(45)-H(45)	120.0
C(47)-C(46)-C(45)	119.7(2)	C(47)-C(46)-H(46)	120.2
C(45)-C(46)-H(46)	120.2	C(46)-C(47)-C(48)	120.4(3)
C(46)-C(47)-H(47)	119.8	C(48)-C(47)-H(47)	119.8
C(43)-C(48)-C(47)	121.0(2)	C(43)-C(48)-H(48)	119.5
C(47)-C(48)-H(48)	119.5	C(50)-C(49)-C(54)	125.1(17)
C(50)-C(49)-H(49)	117.4	C(54)-C(49)-H(49)	117.4
C(49)-C(50)-C(51)	121.3(19)	C(49)-C(50)-H(50)	119.4
C(51)-C(50)-H(50)	119.4	C(52)-C(51)-C(50)	115.5(17)
C(52)-C(51)-H(51)	122.3	C(50)-C(51)-H(51)	122.3
C(51)-C(52)-C(53)	119.1(12)	C(51)-C(52)-H(52)	120.5
C(53)-C(52)-H(52)	120.5	C(54)-C(53)-C(52)	117.5(8)
C(54)-C(53)-H(53)	121.2	C(52)-C(53)-H(53)	121.2
C(53)-C(54)-C(49)	121.5(12)	C(53)-C(54)-H(54)	119.2
C(49)-C(54)-H(54)	119.2	C(60)-C(55)-C(56)	120.0(3)
C(60)-C(55)-H(55)	120.0	C(56)-C(55)-H(55)	120.0
C(55)-C(56)-C(57)	119.6(3)	C(55)-C(56)-H(56)	120.2
C(57)-C(56)-H(56)	120.2	C(58)-C(57)-C(56)	120.1(3)
C(58)-C(57)-H(57)	120.0	C(56)-C(57)-H(57)	120.0
C(59)-C(58)-C(57)	120.0(3)	C(59)-C(58)-H(58)	120.0
C(57)-C(58)-H(58)	120.0	C(58)-C(59)-C(60)	121.0(3)
C(58)-C(59)-H(59)	119.5	C(60)-C(59)-H(59)	119.5
C(55)-C(60)-C(59)	119.3(3)	C(55)-C(60)-H(60)	120.4
C(59)-C(60)-H(60)	120.4	C(50A)-C(49A)-C(54A)	120.0
C(50A)-C(49A)-H(49A)	120.0	C(54A)-C(49A)-H(49A)	120.0
C(51A)-C(50A)-C(49A)	120.0	C(51A)-C(50A)-H(50A)	120.0
C(49A)-C(50A)-H(50A)	120.0	C(50A)-C(51A)-C(52A)	120.0
C(50A)-C(51A)-H(51A)	120.0	C(52A)-C(51A)-H(51A)	120.0

C(53A)-C(52A)-C(51A)	120.0	C(53A)-C(52A)-H(52A)	120.0
C(51A)-C(52A)-H(52A)	120.0	C(54A)-C(53A)-C(52A)	120.0
C(54A)-C(53A)-H(53A)	120.0	C(52A)-C(53A)-H(53A)	120.0
C(53A)-C(54A)-C(49A)	120.0	C(53A)-C(54A)-H(54A)	120.0
C(49A)-C(54A)-H(54A)	120.0		

Table 138. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(ICy)(dppp)(C_5F_4N)H **(82)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	18(1)	18(1)	19(1)	-6(1)	-3(1)	-5(1)
P(1)	20(1)	20(1)	21(1)	-8(1)	-4(1)	-5(1)
P(2)	19(1)	20(1)	22(1)	-6(1)	-4(1)	-5(1)
F(1)	38(1)	33(1)	42(1)	-3(1)	-21(1)	-14(1)
F(2)	41(1)	44(1)	41(1)	2(1)	-25(1)	-8(1)
F(3)	48(1)	25(1)	53(1)	2(1)	-16(1)	-17(1)
F(4)	34(1)	27(1)	36(1)	-6(1)	-14(1)	-11(1)
O(1)	39(1)	36(1)	40(1)	-8(1)	-19(1)	-14(1)
N(1)	23(1)	24(1)	22(1)	-8(1)	-1(1)	-9(1)
N(2)	23(1)	26(1)	23(1)	-8(1)	-1(1)	-9(1)
N(3)	29(1)	28(1)	28(1)	-1(1)	-6(1)	-3(1)
C(1)	24(1)	20(1)	23(1)	-3(1)	-3(1)	-5(1)
C(2)	23(1)	17(1)	21(1)	-5(1)	-4(1)	-7(1)
C(3)	32(1)	33(1)	27(1)	-17(1)	2(1)	-9(1)
C(4)	28(1)	35(1)	28(1)	-15(1)	5(1)	-10(1)
C(5)	29(1)	29(1)	23(1)	-11(1)	1(1)	-15(1)
C(6)	43(2)	27(1)	44(2)	-10(1)	-13(1)	-11(1)
C(7)	63(2)	38(2)	38(2)	-14(1)	-1(1)	-28(1)
C(8)	45(2)	58(2)	42(2)	-25(1)	3(1)	-33(1)
C(9)	32(2)	55(2)	68(2)	-24(2)	-9(1)	-16(1)
C(10)	32(1)	33(1)	46(2)	-13(1)	-11(1)	-10(1)
C(11)	23(1)	26(1)	24(1)	-7(1)	-3(1)	-10(1)
C(12)	31(1)	34(1)	28(1)	-2(1)	-6(1)	-12(1)
C(13)	46(2)	34(1)	39(2)	2(1)	-10(1)	-22(1)
C(14)	37(2)	52(2)	45(2)	-10(1)	-4(1)	-27(1)
C(15)	32(1)	42(2)	52(2)	-8(1)	-17(1)	-13(1)
C(16)	29(1)	34(1)	40(2)	-5(1)	-12(1)	-9(1)
C(17)	19(1)	21(1)	17(1)	-7(1)	0(1)	-4(1)
C(18)	24(1)	25(1)	25(1)	-7(1)	-5(1)	-7(1)
C(19)	26(1)	33(1)	27(1)	-7(1)	-7(1)	-2(1)
C(20)	30(1)	22(1)	31(1)	-6(1)	-2(1)	-10(1)
C(21)	25(1)	26(1)	22(1)	-7(1)	-5(1)	-5(1)
C(22)	24(1)	29(1)	25(1)	-12(1)	-6(1)	-3(1)
C(23)	27(1)	30(1)	21(1)	-6(1)	-4(1)	-6(1)
C(24)	27(1)	22(1)	24(1)	-4(1)	-7(1)	-6(1)
C(25)	20(1)	18(1)	26(1)	-4(1)	-4(1)	-4(1)
C(26)	27(1)	28(1)	28(1)	-9(1)	-3(1)	-7(1)
C(27)	23(1)	37(1)	31(1)	-6(1)	1(1)	-7(1)
C(28)	23(1)	38(1)	36(2)	-1(1)	-8(1)	-11(1)
C(29)	30(1)	37(1)	33(1)	-4(1)	-14(1)	-11(1)
C(30)	25(1)	30(1)	26(1)	-6(1)	-7(1)	-6(1)
C(31)	24(1)	22(1)	21(1)	-8(1)	1(1)	-5(1)
C(32)	28(1)	27(1)	36(1)	-9(1)	-4(1)	-4(1)

C(33)	33(1)	29(1)	45(2)	-4(1)	-5(1)	0(1)
C(34)	43(2)	22(1)	45(2)	-9(1)	4(1)	-6(1)
C(35)	41(2)	30(1)	40(2)	-17(1)	4(1)	-16(1)
C(36)	32(1)	28(1)	28(1)	-12(1)	-2(1)	-6(1)
C(37)	26(1)	23(1)	20(1)	-6(1)	-2(1)	-8(1)
C(38)	29(1)	24(1)	37(1)	-5(1)	-8(1)	-8(1)
C(39)	41(2)	23(1)	41(2)	-6(1)	-6(1)	-9(1)
C(40)	44(2)	33(1)	32(1)	-11(1)	2(1)	-20(1)
C(41)	27(1)	41(2)	37(2)	-15(1)	0(1)	-16(1)
C(42)	27(1)	26(1)	29(1)	-10(1)	-3(1)	-7(1)
C(43)	20(1)	20(1)	27(1)	-5(1)	-5(1)	-5(1)
C(44)	28(1)	25(1)	33(1)	-6(1)	-7(1)	-5(1)
C(45)	31(1)	30(1)	36(2)	-9(1)	1(1)	-1(1)
C(46)	22(1)	38(2)	51(2)	-10(1)	-4(1)	0(1)
C(47)	25(1)	45(2)	52(2)	-14(1)	-16(1)	-2(1)
C(48)	28(1)	33(1)	37(1)	-13(1)	-9(1)	-2(1)
C(49)	112(12)	120(9)	88(9)	-55(7)	48(9)	-77(8)
C(50)	58(7)	74(10)	89(12)	-48(8)	-13(7)	6(6)
C(51)	70(6)	57(6)	62(7)	-34(5)	-26(5)	11(5)
C(52)	45(4)	68(7)	48(5)	-33(6)	1(4)	-3(4)
C(53)	83(7)	41(7)	68(6)	-11(4)	-37(5)	22(5)
C(54)	153(13)	51(6)	61(7)	5(5)	-35(8)	4(7)
C(55)	59(2)	60(2)	56(2)	-24(2)	-15(2)	-26(2)
C(56)	61(2)	70(2)	40(2)	-11(2)	-16(2)	-20(2)
C(57)	61(2)	39(2)	62(2)	-11(2)	-14(2)	-11(2)
C(58)	43(2)	51(2)	76(2)	-37(2)	-19(2)	-2(2)
C(59)	55(2)	65(2)	70(2)	-27(2)	-42(2)	4(2)
C(60)	58(2)	41(2)	68(2)	-12(2)	-23(2)	-7(2)
C(49A)	68(10)	101(18)	123(17)	-80(17)	11(9)	-27(11)
C(50A)	100(14)	28(8)	50(8)	-13(7)	-16(8)	25(8)
C(51A)	450(80)	220(40)	120(30)	-150(30)	150(40)	-260(50)
C(52A)	40(10)	430(100)	90(30)	-170(50)	-4(13)	-10(30)
C(53A)	160(40)	43(16)	41(8)	-11(12)	-10(20)	53(19)
C(54A)	210(40)	63(18)	75(19)	-22(14)	40(20)	-60(20)

Table 139. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Ru(ICy)(dppp)(C_5F_4N)H **(82)**.

Atom	x	y	z	U(eq)
H(3)	258	3155	9504	35
H(4)	-1319	2122	9637	36
H(5)	2812	3130	7778	31
H(6A)	1409	4417	8745	43
H(6B)	1356	4659	7863	43
H(7A)	2722	5641	7980	53
H(7B)	3473	4907	7445	53
H(8A)	4711	4744	8305	52
H(8B)	3553	4484	9029	52
H(9A)	4861	3161	8070	59
H(9B)	4932	2922	8949	59
H(10A)	2782	2739	9371	42
H(10B)	3527	1955	8874	42
H(11)	-321	724	8162	29
H(12A)	-112	-291	9419	38

H(12B)	-1420	335	9782	38
H(13A)	-1778	-1242	9746	48
H(13B)	-1179	-963	8837	48
H(14A)	-3500	124	9542	52
H(14B)	-3397	-614	9029	52
H(15A)	-2367	547	7920	49
H(15B)	-3675	1173	8281	49
H(16A)	-2610	1876	8844	41
H(16B)	-1997	2128	7937	41
H(22A)	4159	1097	4999	30
H(22B)	2684	1096	5375	30
H(23A)	3276	2759	4471	32
H(23B)	3787	2853	5148	32
H(24A)	1211	2657	5374	29
H(24B)	1630	3771	5044	29
H(26)	5999	807	5119	34
H(27)	8028	1165	4831	39
H(28)	8630	1815	5634	40
H(29)	7207	2063	6751	38
H(30)	5155	1709	7050	33
H(32)	5791	-744	6850	37
H(33)	6096	-2554	7217	47
H(34)	4641	-3395	7110	48
H(35)	2853	-2430	6642	43
H(36)	2522	-625	6283	35
H(38)	807	5369	6028	36
H(39)	1860	6759	5705	43
H(40)	4039	6464	5591	42
H(41)	5147	4770	5879	41
H(42)	4092	3367	6273	33
H(44)	-143	3889	7583	35
H(45)	-2281	4620	7856	42
H(46)	-3550	4854	7002	48
H(47)	-2669	4385	5871	48
H(48)	-539	3656	5595	38
H(49)	1185	3321	10780	125
H(50)	826	5011	10337	86
H(51)	2327	6002	10236	73
H(52)	4157	5079	10676	63
H(53)	4423	3256	11119	80
H(54)	2809	2462	11127	115
H(55)	155	-1024	6954	63
H(56)	246	-2740	7725	67
H(57)	-580	-3892	7426	65
H(58)	-1424	-3343	6343	62
H(59)	-1490	-1656	5578	70
H(60)	-686	-485	5866	66
H(49A)	4668	4088	10988	107
H(50A)	3818	2569	11358	79
H(51A)	1873	2640	11097	293
H(52A)	778	4230	10465	207
H(53A)	1627	5748	10095	119
H(54A)	3572	5677	10356	151
H(1)	3203	1897	7419	26(6)

Table 140. Dihedral angles [°] for Ru(ICy)(dppp)(C_5F_4N)H **(82)**.

Atom1 - Atom2 - Atom3 - Atom4	Dihedral
C(1) - Ru(1) - P(1) - C(31)	-70.89(11)
C(2) - Ru(1) - P(1) - C(31)	91.9(2)
C(17) - Ru(1) - P(1) - C(31)	26.01(11)
P(2) - Ru(1) - P(1) - C(31)	-153.48(9)
C(1) - Ru(1) - P(1) - C(25)	168.00(11)
C(2) - Ru(1) - P(1) - C(25)	-29.2(3)
C(17) - Ru(1) - P(1) - C(25)	-95.10(10)
P(2) - Ru(1) - P(1) - C(25)	85.41(9)
C(1) - Ru(1) - P(1) - C(22)	46.54(11)
C(2) - Ru(1) - P(1) - C(22)	-150.7(2)
C(17) - Ru(1) - P(1) - C(22)	143.45(10)
P(2) - Ru(1) - P(1) - C(22)	-36.05(9)
C(1) - Ru(1) - P(2) - C(37)	-177.38(11)
C(2) - Ru(1) - P(2) - C(37)	80.52(10)
C(17) - Ru(1) - P(2) - C(37)	111(2)
P(1) - Ru(1) - P(2) - C(37)	-86.54(9)
C(1) - Ru(1) - P(2) - C(24)	-57.45(10)
C(2) - Ru(1) - P(2) - C(24)	-159.55(10)
C(17) - Ru(1) - P(2) - C(24)	-129(2)
P(1) - Ru(1) - P(2) - C(24)	33.39(8)
C(1) - Ru(1) - P(2) - C(43)	57.77(11)
C(2) - Ru(1) - P(2) - C(43)	-44.33(10)
C(17) - Ru(1) - P(2) - C(43)	-13(2)
P(1) - Ru(1) - P(2) - C(43)	148.61(8)
C(2) - Ru(1) - C(1) - O(1)	129.9(11)
C(17) - Ru(1) - C(1) - O(1)	-142.6(11)
P(1) - Ru(1) - C(1) - O(1)	-54.3(11)
P(2) - Ru(1) - C(1) - O(1)	39.0(11)
C(4) - N(2) - C(2) - N(1)	0.7(2)
C(11) - N(2) - C(2) - N(1)	-177.7(2)
C(4) - N(2) - C(2) - Ru(1)	178.89(16)
C(11) - N(2) - C(2) - Ru(1)	0.5(3)
C(3) - N(1) - C(2) - N(2)	-0.3(2)
C(5) - N(1) - C(2) - N(2)	-179.5(2)
C(3) - N(1) - C(2) - Ru(1)	-178.40(16)
C(5) - N(1) - C(2) - Ru(1)	2.4(3)
C(1) - Ru(1) - C(2) - N(2)	24.6(2)
C(17) - Ru(1) - C(2) - N(2)	-71.7(2)
P(1) - Ru(1) - C(2) - N(2)	-137.82(19)
P(2) - Ru(1) - C(2) - N(2)	107.44(19)
C(1) - Ru(1) - C(2) - N(1)	-157.75(19)
C(17) - Ru(1) - C(2) - N(1)	106.0(2)
P(1) - Ru(1) - C(2) - N(1)	39.9(4)
P(2) - Ru(1) - C(2) - N(1)	-74.86(19)
C(2) - N(1) - C(3) - C(4)	-0.3(3)
C(5) - N(1) - C(3) - C(4)	179.0(2)
N(1) - C(3) - C(4) - N(2)	0.8(3)
C(2) - N(2) - C(4) - C(3)	-1.0(3)
C(11) - N(2) - C(4) - C(3)	177.6(2)
C(2) - N(1) - C(5) - C(10)	-107.3(3)
C(3) - N(1) - C(5) - C(10)	73.5(3)

C(2) - N(1) - C(5) - C(6)	129.4(2)
C(3) - N(1) - C(5) - C(6)	-49.7(3)
N(1) - C(5) - C(6) - C(7)	-179.6(2)
C(10) - C(5) - C(6) - C(7)	56.4(3)
C(5) - C(6) - C(7) - C(8)	-55.1(3)
C(6) - C(7) - C(8) - C(9)	54.3(3)
C(7) - C(8) - C(9) - C(10)	-55.7(3)
C(8) - C(9) - C(10) - C(5)	57.8(3)
N(1) - C(5) - C(10) - C(9)	178.2(2)
C(6) - C(5) - C(10) - C(9)	-57.6(3)
C(2) - N(2) - C(11) - C(12)	119.1(2)
C(4) - N(2) - C(11) - C(12)	-59.2(3)
C(2) - N(2) - C(11) - C(16)	-117.1(2)
C(4) - N(2) - C(11) - C(16)	64.6(3)
N(2) - C(11) - C(12) - C(13)	-179.70(19)
C(16) - C(11) - C(12) - C(13)	56.5(3)
C(11) - C(12) - C(13) - C(14)	-57.2(3)
C(12) - C(13) - C(14) - C(15)	56.5(3)
C(13) - C(14) - C(15) - C(16)	-56.3(3)
C(14) - C(15) - C(16) - C(11)	56.2(3)
N(2) - C(11) - C(16) - C(15)	-179.4(2)
C(12) - C(11) - C(16) - C(15)	-55.8(3)
C(1) - Ru(1) - C(17) - C(18)	178.38(18)
C(2) - Ru(1) - C(17) - C(18)	-79.68(19)
P(1) - Ru(1) - C(17) - C(18)	87.31(18)
P(2) - Ru(1) - C(17) - C(18)	-111(2)
C(1) - Ru(1) - C(17) - C(21)	-1.53(19)
C(2) - Ru(1) - C(17) - C(21)	100.42(18)
P(1) - Ru(1) - C(17) - C(21)	-92.59(17)
P(2) - Ru(1) - C(17) - C(21)	70(2)
C(21) - C(17) - C(18) - F(1)	177.83(19)
Ru(1) - C(17) - C(18) - F(1)	-2.1(3)
C(21) - C(17) - C(18) - C(19)	-1.5(3)
Ru(1) - C(17) - C(18) - C(19)	178.58(17)
C(20) - N(3) - C(19) - F(2)	179.3(2)
C(20) - N(3) - C(19) - C(18)	-0.8(3)
F(1) - C(18) - C(19) - N(3)	-177.6(2)
C(17) - C(18) - C(19) - N(3)	1.8(4)
F(1) - C(18) - C(19) - F(2)	2.3(3)
C(17) - C(18) - C(19) - F(2)	-178.3(2)
C(19) - N(3) - C(20) - F(3)	-179.7(2)
C(19) - N(3) - C(20) - C(21)	-0.3(3)
N(3) - C(20) - C(21) - F(4)	-179.0(2)
F(3) - C(20) - C(21) - F(4)	0.3(3)
N(3) - C(20) - C(21) - C(17)	0.3(4)
F(3) - C(20) - C(21) - C(17)	179.7(2)
C(18) - C(17) - C(21) - F(4)	179.90(18)
Ru(1) - C(17) - C(21) - F(4)	-0.2(3)
C(18) - C(17) - C(21) - C(20)	0.5(3)
Ru(1) - C(17) - C(21) - C(20)	-179.54(17)
C(31) - P(1) - C(22) - C(23)	-176.80(16)
C(25) - P(1) - C(22) - C(23)	-72.74(17)
Ru(1) - P(1) - C(22) - C(23)	59.33(17)
P(1) - C(22) - C(23) - C(24)	-77.6(2)
C(22) - C(23) - C(24) - P(2)	75.6(2)

C(37) - P(2) - C(24) - C(23)	78.15(18)
C(43) - P(2) - C(24) - C(23)	-177.99(16)
Ru(1) - P(2) - C(24) - C(23)	-54.22(18)
C(31) - P(1) - C(25) - C(30)	-112.11(19)
C(22) - P(1) - C(25) - C(30)	142.42(19)
Ru(1) - P(1) - C(25) - C(30)	15.1(2)
C(31) - P(1) - C(25) - C(26)	65.90(19)
C(22) - P(1) - C(25) - C(26)	-39.57(19)
Ru(1) - P(1) - C(25) - C(26)	-166.84(15)
C(30) - C(25) - C(26) - C(27)	-1.1(3)
P(1) - C(25) - C(26) - C(27)	-179.20(18)
C(25) - C(26) - C(27) - C(28)	0.1(4)
C(26) - C(27) - C(28) - C(29)	1.0(4)
C(27) - C(28) - C(29) - C(30)	-1.0(4)
C(26) - C(25) - C(30) - C(29)	1.1(3)
P(1) - C(25) - C(30) - C(29)	179.09(18)
C(28) - C(29) - C(30) - C(25)	0.0(4)
C(25) - P(1) - C(31) - C(32)	27.7(2)
C(22) - P(1) - C(31) - C(32)	132.12(19)
Ru(1) - P(1) - C(31) - C(32)	-104.20(18)
C(25) - P(1) - C(31) - C(36)	-159.37(18)
C(22) - P(1) - C(31) - C(36)	-55.0(2)
Ru(1) - P(1) - C(31) - C(36)	68.70(19)
C(36) - C(31) - C(32) - C(33)	0.3(3)
P(1) - C(31) - C(32) - C(33)	173.31(19)
C(31) - C(32) - C(33) - C(34)	0.1(4)
C(32) - C(33) - C(34) - C(35)	-0.3(4)
C(33) - C(34) - C(35) - C(36)	0.0(4)
C(34) - C(35) - C(36) - C(31)	0.5(4)
C(32) - C(31) - C(36) - C(35)	-0.6(3)
P(1) - C(31) - C(36) - C(35)	-173.79(18)
C(24) - P(2) - C(37) - C(38)	87.0(2)
C(43) - P(2) - C(37) - C(38)	-15.9(2)
Ru(1) - P(2) - C(37) - C(38)	-146.72(17)
C(24) - P(2) - C(37) - C(42)	-88.21(19)
C(43) - P(2) - C(37) - C(42)	168.89(18)
Ru(1) - P(2) - C(37) - C(42)	38.1(2)
C(42) - C(37) - C(38) - C(39)	0.0(4)
P(2) - C(37) - C(38) - C(39)	-175.2(2)
C(37) - C(38) - C(39) - C(40)	2.1(4)
C(38) - C(39) - C(40) - C(41)	-2.2(4)
C(39) - C(40) - C(41) - C(42)	0.2(4)
C(40) - C(41) - C(42) - C(37)	1.9(4)
C(38) - C(37) - C(42) - C(41)	-2.0(3)
P(2) - C(37) - C(42) - C(41)	173.40(18)
C(37) - P(2) - C(43) - C(48)	110.1(2)
C(24) - P(2) - C(43) - C(48)	7.9(2)
Ru(1) - P(2) - C(43) - C(48)	-114.62(19)
C(37) - P(2) - C(43) - C(44)	-69.8(2)
C(24) - P(2) - C(43) - C(44)	-172.01(18)
Ru(1) - P(2) - C(43) - C(44)	65.47(19)
C(48) - C(43) - C(44) - C(45)	0.5(3)
P(2) - C(43) - C(44) - C(45)	-179.60(18)
C(43) - C(44) - C(45) - C(46)	0.0(4)
C(44) - C(45) - C(46) - C(47)	-0.6(4)

C(45) - C(46) - C(47) - C(48)	0.6(4)
C(44) - C(43) - C(48) - C(47)	-0.5(4)
P(2) - C(43) - C(48) - C(47)	179.6(2)
C(46) - C(47) - C(48) - C(43)	-0.1(4)
C(54) - C(49) - C(50) - C(51)	0(4)
C(49) - C(50) - C(51) - C(52)	-1(3)
C(50) - C(51) - C(52) - C(53)	2(2)
C(51) - C(52) - C(53) - C(54)	-0.9(19)
C(52) - C(53) - C(54) - C(49)	-1(2)
C(50) - C(49) - C(54) - C(53)	1(3)
C(60) - C(55) - C(56) - C(57)	-1.1(5)
C(55) - C(56) - C(57) - C(58)	1.0(5)
C(56) - C(57) - C(58) - C(59)	-0.6(5)
C(57) - C(58) - C(59) - C(60)	0.4(5)
C(56) - C(55) - C(60) - C(59)	0.9(5)
C(58) - C(59) - C(60) - C(55)	-0.5(5)
C(54A) - C(49A) - C(50A) - C(51A)	0.0
C(49A) - C(50A) - C(51A) - C(52A)	0.0
C(50A) - C(51A) - C(52A) - C(53A)	0.0
C(51A) - C(52A) - C(53A) - C(54A)	0.0
C(52A) - C(53A) - C(54A) - C(49A)	0.0
C(50A) - C(49A) - C(54A) - C(53A)	0.0

Table 141. Crystal data and structure refinement for Ru(ICy)(dppp)(C_6F_4H)H **(83)**.

Compound	Ru(ICy)(dppp)(C_6F_4H)H **(83)**
Empirical formula	C49 H52 F4 N2 O P2 Ru
Formula weight	923.94
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.7220(1)Å α = 99.060(1)^o
	b = 11.5870(1)Å β = 103.013(1)^o
	c = 19.0110(2)Å γ = 106.890(1)^o
Volume	2138.07(4) Å^3
Z	2
Density (calculated)	1.435 Mg/m^3
Absorption coefficient	0.499 mm^{-1}
F(000)	956
Crystal size	0.35 x 0.30 x 0.30 mm
Theta range for data collection	3.65 to 29.19^o
Index ranges	-14<=h<=14; -15<=k<=15; -26<=l<=26
Reflections collected	40380
Independent reflections	11456 [R(int) = 0.0520]
Reflections observed (>2σ)	10112
Data Completeness	0.989
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.99 and 0.91
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11456 / 1 / 534
Goodness-of-fit on F^2	1.025
Final R indices [I>2σ(I)]	R1 = 0.0324 wR2 = 0.0761
R indices (all data)	R1 = 0.0397 wR2 = 0.0801
Largest diff. peak and hole	0.584 and -0.803 eÅ^{-3}

Table 142. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Ru(ICy)(dppp)(C_6F_4H)H **(83)**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Ru(1)	5031(1)	5629(1)	7343(1)	15(1)
P(1)	5198(1)	3661(1)	7167(1)	18(1)
P(2)	7088(1)	6441(1)	7095(1)	18(1)
F(1)	4266(1)	5402(1)	8976(1)	29(1)
F(2)	2044(1)	4292(1)	9293(1)	36(1)
F(3)	-406(1)	2995(1)	6758(1)	34(1)
F(4)	1750(1)	4160(1)	6400(1)	28(1)
O(1)	3840(1)	4952(1)	5655(1)	29(1)
N(1)	4378(2)	8138(1)	7326(1)	19(1)
N(2)	5453(2)	8193(1)	8438(1)	20(1)
C(1)	4187(2)	5259(2)	6296(1)	21(1)
C(2)	4960(2)	7447(2)	7725(1)	17(1)
C(3)	4501(2)	9250(2)	7770(1)	26(1)
C(4)	5172(2)	9289(2)	8460(1)	27(1)
C(5)	3649(2)	7777(2)	6528(1)	21(1)
C(6)	2134(2)	7138(2)	6393(1)	29(1)
C(7)	1406(2)	6694(2)	5557(1)	39(1)
C(8)	1697(3)	7764(2)	5170(1)	41(1)
C(9)	3218(3)	8420(2)	5335(1)	40(1)
C(10)	3906(2)	8886(2)	6174(1)	28(1)
C(11)	6237(2)	7979(2)	9119(1)	20(1)
C(12)	5647(2)	8237(2)	9763(1)	33(1)
C(13)	6434(3)	7968(2)	10459(1)	41(1)
C(14)	7940(3)	8711(2)	10672(1)	45(1)
C(15)	8528(2)	8482(2)	10024(1)	37(1)
C(16)	7742(2)	8755(2)	9326(1)	30(1)
C(17)	3191(2)	4862(1)	7654(1)	18(1)
C(18)	3137(2)	4834(2)	8380(1)	22(1)
C(19)	1978(2)	4247(2)	8566(1)	26(1)
C(20)	753(2)	3624(2)	8036(1)	28(1)
C(21)	762(2)	3623(2)	7316(1)	25(1)
C(22)	1924(2)	4234(2)	7142(1)	21(1)
C(23)	5912(2)	3269(2)	6403(1)	23(1)
C(24)	7336(2)	4162(2)	6485(1)	25(1)
C(25)	7348(2)	5425(2)	6332(1)	23(1)
C(26)	6176(2)	3224(2)	7944(1)	20(1)
C(27)	6777(2)	2318(2)	7831(1)	25(1)
C(28)	7464(2)	1973(2)	8428(1)	30(1)
C(29)	7562(2)	2522(2)	9147(1)	31(1)
C(30)	6952(2)	3406(2)	9268(1)	35(1)
C(31)	6272(2)	3757(2)	8673(1)	29(1)
C(32)	3583(2)	2354(2)	6884(1)	21(1)
C(33)	3111(2)	1732(2)	7395(1)	25(1)
C(34)	1865(2)	774(2)	7171(1)	32(1)
C(35)	1079(2)	419(2)	6437(1)	34(1)
C(36)	1523(2)	1052(2)	5932(1)	34(1)
C(37)	2754(2)	2013(2)	6150(1)	29(1)
C(38)	8721(2)	6770(2)	7794(1)	22(1)
C(39)	9951(2)	7356(2)	7660(1)	32(1)

C(40)	11179(2)	7478(2)	8152(1)	39(1)
C(41)	11199(2)	7010(2)	8777(1)	36(1)
C(42)	9991(2)	6430(2)	8919(1)	33(1)
C(43)	8757(2)	6320(2)	8432(1)	27(1)
C(44)	7345(2)	7876(2)	6764(1)	20(1)
C(45)	6817(2)	7834(2)	6016(1)	27(1)
C(46)	6985(2)	8921(2)	5767(1)	30(1)
C(47)	7683(2)	10063(2)	6260(1)	28(1)
C(48)	8206(2)	10122(2)	7004(1)	28(1)
C(49)	8021(2)	9036(2)	7250(1)	26(1)

Table 143. Bond lengths [Å] and angles [°] for Ru(ICy)(dppp)(C_6F_4H)H **(83)**.

Ru(1)-C(1)	1.9139(17)	Ru(1)-C(2)	2.1467(16)
Ru(1)-C(17)	2.1694(16)	Ru(1)-P(1)	2.3167(4)
Ru(1)-P(2)	2.3179(4)	P(1)-C(32)	1.8382(18)
P(1)-C(26)	1.8405(17)	P(1)-C(23)	1.8422(17)
P(2)-C(44)	1.8380(17)	P(2)-C(38)	1.8394(18)
P(2)-C(25)	1.8449(17)	F(1)-C(18)	1.367(2)
F(2)-C(19)	1.360(2)	F(3)-C(21)	1.360(2)
F(4)-C(22)	1.365(2)	O(1)-C(1)	1.153(2)
N(1)-C(2)	1.370(2)	N(1)-C(3)	1.378(2)
N(1)-C(5)	1.471(2)	N(2)-C(2)	1.381(2)
N(2)-C(4)	1.384(2)	N(2)-C(11)	1.475(2)
C(3)-C(4)	1.334(3)	C(5)-C(6)	1.519(3)
C(5)-C(10)	1.526(2)	C(6)-C(7)	1.533(3)
C(7)-C(8)	1.529(3)	C(8)-C(9)	1.520(4)
C(9)-C(10)	1.532(3)	C(11)-C(16)	1.525(3)
C(11)-C(12)	1.528(2)	C(12)-C(13)	1.529(3)
C(13)-C(14)	1.517(4)	C(14)-C(15)	1.525(3)
C(15)-C(16)	1.535(3)	C(17)-C(22)	1.390(2)
C(17)-C(18)	1.398(2)	C(18)-C(19)	1.384(2)
C(19)-C(20)	1.373(3)	C(20)-C(21)	1.370(3)
C(21)-C(22)	1.381(3)	C(23)-C(24)	1.533(3)
C(24)-C(25)	1.533(2)	C(26)-C(31)	1.393(2)
C(26)-C(27)	1.396(2)	C(27)-C(28)	1.388(3)
C(28)-C(29)	1.382(3)	C(29)-C(30)	1.383(3)
C(30)-C(31)	1.387(3)	C(32)-C(33)	1.395(3)
C(32)-C(37)	1.399(2)	C(33)-C(34)	1.390(3)
C(34)-C(35)	1.384(3)	C(35)-C(36)	1.382(3)
C(36)-C(37)	1.381(3)	C(38)-C(43)	1.390(2)
C(38)-C(39)	1.396(3)	C(39)-C(40)	1.388(3)
C(40)-C(41)	1.379(3)	C(41)-C(42)	1.383(3)
C(42)-C(43)	1.393(3)	C(44)-C(49)	1.387(2)
C(44)-C(45)	1.395(2)	C(45)-C(46)	1.392(3)
C(46)-C(47)	1.380(3)	C(47)-C(48)	1.382(3)
C(48)-C(49)	1.388(2)		
C(1)-Ru(1)-C(2)	102.80(7)	C(1)-Ru(1)-C(17)	96.83(7)
C(2)-Ru(1)-C(17)	88.36(6)	C(1)-Ru(1)-P(1)	87.68(5)
C(2)-Ru(1)-P(1)	169.16(4)	C(17)-Ru(1)-P(1)	87.63(4)
C(1)-Ru(1)-P(2)	87.19(5)	C(2)-Ru(1)-P(2)	92.02(4)
C(17)-Ru(1)-P(2)	175.77(4)	P(1)-Ru(1)-P(2)	91.247(16)
C(32)-P(1)-C(26)	100.63(8)	C(32)-P(1)-C(23)	100.38(8)
C(26)-P(1)-C(23)	103.36(8)	C(32)-P(1)-Ru(1)	116.09(6)

C(26)-P(1)-Ru(1)	119.35(6)	C(23)-P(1)-Ru(1)	114.35(6)
C(44)-P(2)-C(38)	102.65(8)	C(44)-P(2)-C(25)	100.47(8)
C(38)-P(2)-C(25)	98.47(8)	C(44)-P(2)-Ru(1)	116.29(6)
C(38)-P(2)-Ru(1)	121.49(6)	C(25)-P(2)-Ru(1)	114.10(6)
C(2)-N(1)-C(3)	111.78(14)	C(2)-N(1)-C(5)	126.68(14)
C(3)-N(1)-C(5)	121.50(14)	C(2)-N(2)-C(4)	111.04(14)
C(2)-N(2)-C(11)	128.86(14)	C(4)-N(2)-C(11)	120.05(14)
O(1)-C(1)-Ru(1)	168.84(15)	N(1)-C(2)-N(2)	102.80(13)
N(1)-C(2)-Ru(1)	128.60(11)	N(2)-C(2)-Ru(1)	128.57(12)
C(4)-C(3)-N(1)	107.17(15)	C(3)-C(4)-N(2)	107.20(15)
N(1)-C(5)-C(6)	111.19(14)	N(1)-C(5)-C(10)	111.70(14)
C(6)-C(5)-C(10)	110.64(15)	C(5)-C(6)-C(7)	110.41(17)
C(8)-C(7)-C(6)	111.20(17)	C(9)-C(8)-C(7)	111.12(17)
C(8)-C(9)-C(10)	111.15(18)	C(5)-C(10)-C(9)	108.59(16)
N(2)-C(11)-C(16)	111.54(14)	N(2)-C(11)-C(12)	110.81(15)
C(16)-C(11)-C(12)	110.77(15)	C(11)-C(12)-C(13)	110.42(17)
C(14)-C(13)-C(12)	111.44(18)	C(13)-C(14)-C(15)	111.10(17)
C(14)-C(15)-C(16)	111.49(19)	C(11)-C(16)-C(15)	110.00(15)
C(22)-C(17)-C(18)	111.23(15)	C(22)-C(17)-Ru(1)	123.48(12)
C(18)-C(17)-Ru(1)	125.07(12)	F(1)-C(18)-C(19)	114.03(15)
F(1)-C(18)-C(17)	121.37(15)	C(19)-C(18)-C(17)	124.61(16)
F(2)-C(19)-C(20)	118.79(16)	F(2)-C(19)-C(18)	119.39(17)
C(20)-C(19)-C(18)	121.81(17)	C(21)-C(20)-C(19)	115.50(17)
F(3)-C(21)-C(20)	118.86(16)	F(3)-C(21)-C(22)	119.28(17)
C(20)-C(21)-C(22)	121.86(17)	F(4)-C(22)-C(21)	114.34(15)
F(4)-C(22)-C(17)	120.70(15)	C(21)-C(22)-C(17)	124.96(16)
C(24)-C(23)-P(1)	114.36(12)	C(23)-C(24)-C(25)	113.76(15)
C(24)-C(25)-P(2)	113.05(12)	C(31)-C(26)-C(27)	117.93(16)
C(31)-C(26)-P(1)	119.81(14)	C(27)-C(26)-P(1)	122.17(13)
C(28)-C(27)-C(26)	120.90(17)	C(29)-C(28)-C(27)	120.41(18)
C(28)-C(29)-C(30)	119.35(18)	C(29)-C(30)-C(31)	120.35(18)
C(30)-C(31)-C(26)	121.05(18)	C(33)-C(32)-C(37)	118.32(17)
C(33)-C(32)-P(1)	121.74(13)	C(37)-C(32)-P(1)	119.83(14)
C(34)-C(33)-C(32)	120.54(18)	C(35)-C(34)-C(33)	120.37(19)
C(36)-C(35)-C(34)	119.42(19)	C(37)-C(36)-C(35)	120.61(19)
C(36)-C(37)-C(32)	120.67(19)	C(43)-C(38)-C(39)	118.57(17)
C(43)-C(38)-P(2)	120.23(14)	C(39)-C(38)-P(2)	120.84(14)
C(40)-C(39)-C(38)	120.55(18)	C(41)-C(40)-C(39)	120.26(19)
C(40)-C(41)-C(42)	120.01(18)	C(41)-C(42)-C(43)	119.87(18)
C(38)-C(43)-C(42)	120.73(18)	C(49)-C(44)-C(45)	117.76(15)
C(49)-C(44)-P(2)	121.48(12)	C(45)-C(44)-P(2)	120.71(13)
C(46)-C(45)-C(44)	120.83(17)	C(47)-C(46)-C(45)	120.30(18)
C(46)-C(47)-C(48)	119.63(17)	C(47)-C(48)-C(49)	119.81(17)
C(44)-C(49)-C(48)	121.65(12)		

Table 144. Anisotropic displacement parameters ($Å^2$ x 10^3) for Ru(ICy)(dppp)(C_6F_4H)H **(83)**. The anisotropic displacement factor exponent takes the form: -2 gpi^2 [h^2 a^{*2} U11 + ... + 2 h k a* b* U

Atom	U11	U22	U33	U23	U13	U12
Ru(1)	18(1)	15(1)	13(1)	4(1)	4(1)	6(1)
P(1)	23(1)	16(1)	14(1)	3(1)	4(1)	8(1)
P(2)	19(1)	21(1)	15(1)	6(1)	6(1)	8(1)
F(1)	25(1)	33(1)	18(1)	2(1)	5(1)	-2(1)

F(2)	38(1)	40(1)	26(1)	5(1)	18(1)	1(1)
F(3)	18(1)	38(1)	37(1)	3(1)	0(1)	5(1)
F(4)	25(1)	34(1)	20(1)	6(1)	2(1)	8(1)
O(1)	37(1)	32(1)	16(1)	5(1)	3(1)	13(1)
N(1)	23(1)	18(1)	16(1)	4(1)	4(1)	9(1)
N(2)	24(1)	18(1)	17(1)	4(1)	4(1)	6(1)
C(1)	23(1)	19(1)	22(1)	7(1)	6(1)	9(1)
C(2)	16(1)	17(1)	17(1)	3(1)	6(1)	4(1)
C(3)	36(1)	19(1)	24(1)	3(1)	4(1)	13(1)
C(4)	39(1)	18(1)	22(1)	0(1)	5(1)	11(1)
C(5)	26(1)	22(1)	17(1)	6(1)	5(1)	12(1)
C(6)	27(1)	31(1)	25(1)	6(1)	3(1)	7(1)
C(7)	35(1)	42(1)	28(1)	-5(1)	-7(1)	13(1)
C(8)	58(1)	49(1)	19(1)	2(1)	-3(1)	35(1)
C(9)	64(2)	43(1)	22(1)	14(1)	11(1)	27(1)
C(10)	38(1)	29(1)	23(1)	12(1)	9(1)	15(1)
C(11)	24(1)	19(1)	15(1)	3(1)	3(1)	4(1)
C(12)	41(1)	42(1)	22(1)	9(1)	13(1)	19(1)
C(13)	55(1)	56(1)	19(1)	14(1)	14(1)	25(1)
C(14)	60(2)	43(1)	19(1)	2(1)	-8(1)	15(1)
C(15)	28(1)	41(1)	31(1)	13(1)	-5(1)	2(1)
C(16)	26(1)	30(1)	26(1)	9(1)	2(1)	2(1)
C(17)	21(1)	13(1)	20(1)	4(1)	8(1)	7(1)
C(18)	21(1)	18(1)	23(1)	1(1)	6(1)	4(1)
C(19)	30(1)	22(1)	26(1)	5(1)	14(1)	7(1)
C(20)	23(1)	25(1)	35(1)	5(1)	14(1)	4(1)
C(21)	17(1)	20(1)	32(1)	2(1)	3(1)	6(1)
C(22)	23(1)	19(1)	22(1)	4(1)	6(1)	9(1)
C(23)	34(1)	23(1)	17(1)	4(1)	9(1)	15(1)
C(24)	33(1)	29(1)	22(1)	6(1)	13(1)	18(1)
C(25)	28(1)	27(1)	19(1)	7(1)	12(1)	12(1)
C(26)	21(1)	18(1)	18(1)	7(1)	4(1)	5(1)
C(27)	28(1)	28(1)	22(1)	8(1)	8(1)	13(1)
C(28)	30(1)	35(1)	33(1)	16(1)	11(1)	18(1)
C(29)	33(1)	31(1)	25(1)	13(1)	1(1)	8(1)
C(30)	55(1)	28(1)	19(1)	5(1)	4(1)	13(1)
C(31)	43(1)	25(1)	21(1)	5(1)	7(1)	15(1)
C(32)	23(1)	15(1)	22(1)	0(1)	3(1)	8(1)
C(33)	26(1)	22(1)	25(1)	3(1)	6(1)	9(1)
C(34)	27(1)	27(1)	40(1)	4(1)	15(1)	7(1)
C(35)	23(1)	27(1)	43(1)	-4(1)	6(1)	5(1)
C(36)	29(1)	30(1)	31(1)	-3(1)	-4(1)	9(1)
C(37)	32(1)	25(1)	24(1)	2(1)	1(1)	9(1)
C(38)	20(1)	26(1)	20(1)	5(1)	6(1)	10(1)
C(39)	22(1)	49(1)	27(1)	14(1)	9(1)	11(1)
C(40)	20(1)	61(2)	34(1)	13(1)	9(1)	11(1)
C(41)	23(1)	56(1)	27(1)	7(1)	1(1)	16(1)
C(42)	29(1)	43(1)	25(1)	13(1)	1(1)	12(1)
C(43)	24(1)	33(1)	23(1)	9(1)	5(1)	9(1)
C(44)	20(1)	23(1)	21(1)	10(1)	10(1)	8(1)
C(45)	31(1)	25(1)	23(1)	8(1)	4(1)	8(1)
C(46)	37(1)	30(1)	24(1)	13(1)	7(1)	11(1)
C(47)	32(1)	27(1)	30(1)	14(1)	13(1)	11(1)
C(48)	36(1)	22(1)	26(1)	5(1)	13(1)	8(1)
C(49)	35(1)	27(1)	18(1)	8(1)	11(1)	10(1)

Table 145. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for Ru(ICy)(dppp)(C_6F_4H)H **(83)**.

Atom	x	y	z	U(eq)
H(3)	4171	9873	7614	31
H(4)	5412	9946	8888	33
H(5)	4005	7167	6279	25
H(6A)	1749	7724	6628	35
H(6B)	1985	6419	6623	35
H(7A)	1715	6035	5333	47
H(7B)	413	6335	5478	47
H(8A)	1286	7437	4627	50
H(8B)	1273	8367	5342	50
H(9A)	3376	9132	5099	48
H(9B)	3628	7839	5120	48
H(10A)	4896	9302	6271	34
H(10B)	3529	9495	6392	34
H(11)	6159	7083	9019	24
H(12A)	4677	7708	9624	39
H(12B)	5698	9116	9869	39
H(13A)	6067	8177	10877	49
H(13B)	6307	7071	10366	49
H(14A)	8429	8473	11101	54
H(14B)	8077	9607	10823	54
H(15A)	8490	7607	9912	45
H(15B)	9495	9019	10167	45
H(16A)	7850	9649	9420	36
H(16B)	8114	8557	8908	36
H(20)	-48	3221	8159	33
H(23A)	5952	2420	6372	28
H(23B)	5289	3261	5929	28
H(24A)	7740	3769	6138	31
H(24B)	7916	4298	6996	31
H(25A)	6622	5289	5869	28
H(25B)	8230	5850	6251	28
H(27)	6716	1932	7339	30
H(28)	7869	1356	8341	36
H(29)	8043	2293	9556	37
H(30)	7000	3775	9760	42
H(31)	5865	4371	8763	35
H(33)	3646	1966	7899	30
H(34)	1551	360	7524	38
H(35)	241	-253	6281	40
H(36)	976	824	5430	41
H(37)	3041	2446	5798	34
H(39)	9946	7673	7229	38
H(40)	12011	7885	8058	47
H(41)	12042	7088	9109	43
H(42)	10004	6106	9349	40
H(43)	7930	5933	8536	32
H(45)	6338	7053	5672	32
H(46)	6617	8877	5256	36
H(47)	7804	10803	6088	33
H(48)	8691	10904	7345	34

H(49)	8364	9087	7765	31
H(1)	5844	5767	8188	33(6)